

# Topology of Andreev Bound States with Flat Dispersion

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## Abstract

A theory of dispersionless Andreev bound states on surfaces of time-reversal invariant unconventional superconductors is presented. The generalized criterion for the dispersionless Andreev bound state is derived from the bulk-edge correspondence, and the chiral spin structure of the dispersionless Andreev bound states is argued from which the Andreev bound state is stabilized. Then we summarize the criterion in a form of index theorems. The index theorems are proved in a general framework to certify the bulk-edge correspondence. As concrete examples, we discuss (i)  $d_{xy}$ -wave superconductor (ii)  $p_x$ -wave superconductor, and (iii) noncentrosymmetric superconductors. In the last example, we find a peculiar time-reversal invariant Majorana fermion. The time-reversal invariant Majorana fermion shows an unusual response to the Zeeman magnetic field, which can be used to identify it experimentally.

## I. INTRODUCTION

In unconventional superconductors, due to the sign change of the pair potential on the Fermi surface it is known that an Andreev bound state (ABS) via Andreev reflection<sup>1-3</sup> is generated at a surface of superconductors<sup>4-9</sup>. The ABS shows up as a zero bias conductance peak of tunneling spectroscopy<sup>6-8,10</sup>, and through the study of tunneling spectroscopy of high  $T_c$  cuprates<sup>11-20</sup>, it has been established that a dispersionless zero energy ABS<sup>7</sup> is generated for  $d_{xy}$ -wave superconductors. The existence of the ABS influences seriously interface and surface properties<sup>21-26</sup>. Great amount of unconventional quantum phenomena appear in quasiparticle tunneling<sup>10,27,28</sup>, Josephson effect<sup>29-34</sup>, spin transport phenomena<sup>35,36</sup>, Meissner effect<sup>37-40</sup> and macroscopic quantum tunneling<sup>41-43</sup>.

Dispersionless ABSs appear not only in spin-singlet  $d_{xy}$ -wave superconductors, but also in spin-triplet  $p_x$ -wave ones<sup>4,5,7</sup>. However, it has been shown that the proximity effect of the ABS is completely different in these superconductors<sup>44-48</sup>. In the latter case, the ABS can penetrate into a diffusive normal metal (DN) attached to the superconductor, while it is not possible in the former one. The underlying physics is the existence of odd-frequency pairings<sup>49</sup>: Odd-frequency pairings are induced on boundaries of superconductors due to the breakdown of the translational invariance<sup>50</sup>. From the requirement of the Fermi statistics, the ABS in  $d_{xy}$ -wave superconductors is expressed by an odd-frequency spin-singlet odd-parity state, but the ABS in  $p_x$ -wave superconductors an odd-frequency spin-triplet even-parity one<sup>51,52</sup>. Then the ABS in  $p_x$ -wave superconductors can penetrate in DN since the odd-frequency spin-triplet  $s$ -wave component in  $p_x$ -wave superconductors is robust against impurity scattering<sup>40,49,51,53,54</sup>.

Another important character of ABSs is that they realize Majorana fermions in condensed matter systems. For time-reversal breaking superconductors, ABSs with linear dispersion have been studied in the context of the chiral  $p$ -wave superconductor such as  $\text{Sr}_2\text{RuO}_4$ <sup>55-58</sup>. In this case, the ABSs are an analogous state to the edge modes of quantum Hall system (QHS)<sup>59,60</sup>, which induce a spontaneous charge current along the edge<sup>61,62</sup>. The main difference between the edge state of QHS and the ABS is that the latter excitation is a Majorana fermion realizing a non-Abelian anyon, which can be used in a fault tolerant topological quantum computation<sup>63,64</sup>. In addition to spin-triplet superconductors<sup>60,65-67</sup>, now it has been known that spin-singlet superconducting states may support a non-Abelian anyon<sup>68-74</sup>,

and the various unusual transport properties have been explored<sup>60,65,69–86</sup>. For time-reversal invariant superconductors, the ABS with linear dispersion have been studied mainly in the context of non-centrosymmetric (NCS) superconductors<sup>87–91</sup>. One of the remarkable features of the NCS superconductors is that the superconducting pair potential becomes a mixture of spin-singlet even-parity and spin-triplet odd-parity ones<sup>92</sup>, and for CePt<sub>3</sub>Si<sup>93</sup>, the ABS and the relevant charge transport properties<sup>66,94–101</sup> have been studied based on  $s + p$ -wave pairing. The resulting ABS has two linear dispersions analogous to helical edge modes<sup>66</sup>, in Quantum spin Hall systems (QSHS)<sup>102–105</sup>, thus instead of charge current, spin current is spontaneously generated along the edge. The ABS forms a Kramers pair of Majorana modes called a helical Majorana edge mode, and several new features of spin and charge transport stemming from these helical Majorana edge modes have been predicted<sup>66,97–100,106</sup>.

It has been found recently that Majorana fermions are possible also for ABSs with flat dispersion<sup>107,108</sup>. Although  $s + p$ -wave superconducting states have been studied intensively, other types of NCS pairing symmetry may appear in strongly correlated systems. Microscopic calculations have shown that a parity mixed pairing state between the spin-singlet  $d_{x^2-y^2}$ -wave pairing and the spin-triplet  $f$ -wave one is realized in the Hubbard model near the half filling<sup>109–112</sup>. Moreover, a gap function which consists of the spin-singlet  $d_{xy}$ -wave component and spin-triplet  $p$ -wave one has been proposed,<sup>113</sup> as a possible candidate of superconductivity generated at heterointerface LaAlO<sub>3</sub>/SrTiO<sub>3</sub><sup>91</sup>. Examining the ABSs in these NCS superconductors,<sup>107,108</sup> we found a new type of ABS in the  $d_{xy} + p$ -wave NCS superconductor<sup>114</sup>: Due to the Fermi surface splitting by the spin-orbit coupling, there appears a single branch of Majorana edge state with flat dispersion preserving the time reversal symmetry. A similar ABS with flat band in NCS superconductors was also discussed in Ref.<sup>115</sup>.

In this paper, we will address topological properties of the dispersionless ABSs on surfaces of time-reversal invariant superconductors. For the ABSs with linear dispersion, it has been known that their presence is guaranteed by the topological invariance defined in bulk Hamiltonian. For instance, for full gapped two dimensional time-reversal breaking (invariant) superconductors, a non-zero Chern number<sup>116,117</sup> (non-trivial  $\mathbf{Z}_2$  topological number<sup>102,103</sup>) ensures the existence of the Majorana fermions<sup>59,60,118–124</sup>, and for nodal superconductors, the parity of Chern number ensures the existence of Majorana fermions<sup>74</sup>. Furthermore, for spin-triplet superconductors, the ABSs on the boundary can be predicted

from the topology of the Fermi surface<sup>67,123,125</sup>. However, Majorana edge mode with flat dispersion and its relevance to the symmetry of Hamiltonian has not been clarified yet. It is an interesting issue to clarify the relevance of the topological property to the wave function of ABS with flat dispersion.

The organization of this paper as follows. In section II, we will define a topological number starting from the bulk Bogoliubov de Gennes (BdG) Hamiltonian, and present a topological criterion for dispersionless ABSs. In section III, we discuss topological stability of the ABSs using the chiral symmetry of time-reversal invariant BdG Hamiltonians. Then, we propose index theorems for the dispersionless ABSs. In section IV, the relation between the sign change of gap function and topological criterion will be discussed. We will show that the sign change of the pair potential is directly relevant to the index theorem we proposed. As concrete examples, we will discuss the ABSs in spin-singlet  $d_{xy}$ -wave superconductors and spin triplet  $p_x$ -wave ones, respectively. By constructing the wave function of the ABS explicitly, the index theorems are confirmed. We also find that the topological structures of the ABSs are consistent with those of the odd-frequency pairings. In section V, we will apply our theory to the ABSs in noncentrosymmetric superconductors, in which a Majorana fermion with flat dispersion is realized. The wave function of the ABS for  $d_{xy} + p$ -wave superconductors will be derived, and the relevant topological number will be discussed. It will be also found that the Majorana fermion has an anisotropic response to Zeeman magnetic field, which can be explained by a  $Z_2$  topological number. In section VI, we will finally provide a general framework to certify the bulk-edge correspondence, and by using it the index theorems will be proved. In section VII, we will summarize our results, and discuss possible application of our theory to other systems. Throughout this paper, we use a convention of  $\hbar = 1$  except in Sec.VI.

## II. TOPOLOGICAL CRITERION FOR DISPERSIONLESS ANDREEV BOUND STATE

We start with a general BdG Hamiltonian for superconducting states.

$$\mathcal{H} = \frac{1}{2} \sum_{\mathbf{k}\alpha\alpha'} \begin{pmatrix} c_{\mathbf{k}\alpha}^\dagger & c_{-\mathbf{k}\alpha} \end{pmatrix} \mathcal{H}(\mathbf{k}) \begin{pmatrix} c_{\mathbf{k}\alpha'} \\ c_{-\mathbf{k}\alpha'}^\dagger \end{pmatrix}, \quad (1)$$

with

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} \hat{\mathcal{E}}(\mathbf{k})_{\alpha\alpha'} & \hat{\Delta}(\mathbf{k})_{\alpha\alpha'} \\ \hat{\Delta}^\dagger(\mathbf{k})_{\alpha\alpha'} & -\hat{\mathcal{E}}^T(-\mathbf{k})_{\alpha\alpha'} \end{pmatrix}, \quad (2)$$

where  $c_{\mathbf{k}\alpha}^\dagger$  ( $c_{\mathbf{k}\alpha}$ ) denotes the creation (annihilation) operator of electron with momentum  $\mathbf{k}$ . The suffix  $\alpha$  labels other degrees of freedom for electron such as spin, orbital degrees of freedom, sublattice indices, and so on.  $\hat{\mathcal{E}}(\mathbf{k})$  is the Hermitian matrix describing the normal dispersion of electron, and  $\hat{\Delta}(\mathbf{k})$  the gap function which satisfies  $\hat{\Delta}^T(-\mathbf{k}) = -\hat{\Delta}(\mathbf{k})$ .

In the following, we suppose time-reversal invariant superconducting states. The time-reversal operation for electron is given by the antiunitary operator  $\mathcal{T}$  in the form,

$$\mathcal{T} = UK, \quad (3)$$

where  $U$  is a constant unitary matrix acting on the suffix  $\alpha$  of electron, and  $K$  the complex conjugate operator.  $K$  also reverses the sign of the momentum  $\mathbf{k}$ .  $U$  satisfies  $UU^* = -1$  since  $\mathcal{T}^2 = -1$  for electron. Then, for time-reversal invariant superconductors, the BdG Hamiltonian  $\mathcal{H}(\mathbf{k})$  satisfies,

$$\Theta \mathcal{H}(\mathbf{k}) \Theta^{-1} = \mathcal{H}^*(-\mathbf{k}), \quad \Theta = \begin{pmatrix} U_{\alpha\alpha'} & 0 \\ 0 & U_{\alpha\alpha'}^* \end{pmatrix}, \quad (4)$$

which implies

$$U \hat{\mathcal{E}}(\mathbf{k}) U^\dagger = \hat{\mathcal{E}}^*(-\mathbf{k}), \quad U \hat{\Delta}(\mathbf{k}) U^T = \hat{\Delta}^*(-\mathbf{k}). \quad (5)$$

In addition, the BdG Hamiltonian  $\mathcal{H}(\mathbf{k})$  has the following particle-hole symmetry,

$$\mathcal{C} \mathcal{H}(\mathbf{k}) \mathcal{C}^{-1} = -\mathcal{H}^*(-\mathbf{k}), \quad \mathcal{C} = \begin{pmatrix} 0 & \delta_{\alpha\alpha'} \\ \delta_{\alpha\alpha'} & 0 \end{pmatrix}. \quad (6)$$

Therefore, combining with (4) and (6), we obtain the so-called chiral symmetry

$$\{\Gamma, \mathcal{H}(\mathbf{k})\} = 0, \quad \Gamma = -i\mathcal{C}\Theta = \begin{pmatrix} 0 & -iU_{\alpha\alpha'}^* \\ -iU_{\alpha\alpha'} & 0 \end{pmatrix}, \quad (7)$$

which is the central ingredient of our theory. For later convenience, we perform here the following unitary transformation by which  $\Gamma$  is diagonalized

$$U_\Gamma^\dagger \Gamma U_\Gamma = \begin{pmatrix} \delta_{\alpha\alpha'} & 0 \\ 0 & -\delta_{\alpha\alpha'} \end{pmatrix}, \quad U_\Gamma = \frac{1}{\sqrt{2}} \begin{pmatrix} \delta_{\alpha\alpha'} & iU_{\alpha\alpha'}^\dagger \\ -iU_{\alpha\alpha'} & -\delta_{\alpha\alpha'} \end{pmatrix}. \quad (8)$$

Then the BdG Hamiltonian becomes off-diagonal,

$$U_{\Gamma}^{\dagger} \mathcal{H}(\mathbf{k}) U_{\Gamma} = \begin{pmatrix} 0 & \hat{q}(\mathbf{k}) \\ \hat{q}^{\dagger}(\mathbf{k}) & 0 \end{pmatrix}, \quad (9)$$

with

$$\hat{q}(\mathbf{k}) = i\hat{\mathcal{E}}(\mathbf{k})U^{\dagger} - \hat{\Delta}(\mathbf{k}). \quad (10)$$

Now consider the ABS on a surface of the superconductor. The relevant topological number for the flat dispersion (or dispersionless) ABS is

$$\begin{aligned} W(\mathbf{k}_{\parallel}) &= -\frac{1}{4\pi i} \int d\mathbf{k}_{\perp} \text{tr}[\Gamma \mathcal{H}^{-1}(\mathbf{k}) \partial_{\mathbf{k}_{\perp}} \mathcal{H}(\mathbf{k})] \\ &= \frac{1}{4\pi i} \int d\mathbf{k}_{\perp} \text{tr}[\hat{q}^{-1}(\mathbf{k}) \partial_{\mathbf{k}_{\perp}} \hat{q}(\mathbf{k}) - \hat{q}^{\dagger-1}(\mathbf{k}) \partial_{\mathbf{k}_{\perp}} \hat{q}^{\dagger}(\mathbf{k})] \\ &= \frac{1}{2\pi} \text{Im} \left[ \int d\mathbf{k}_{\perp} \partial_{\mathbf{k}_{\perp}} \ln \det \hat{q}(\mathbf{k}) \right], \end{aligned} \quad (11)$$

where  $\mathbf{k}_{\parallel}$  ( $\mathbf{k}_{\perp}$ ) is the momentum parallel (perpendicular) to the surface we consider, and the integration is along the  $\mathbf{k}_{\perp}$ -direction with fixing the value of  $\mathbf{k}_{\parallel}$  (Fig.1). For instance, for the surface perpendicular to the  $x$  direction,  $\mathbf{k}_{\perp} = k_x$  and  $\mathbf{k}_{\parallel} = (k_y, k_z)$ .

For superfluids or continuum models of superconductors, the line integral in (11) is performed from  $\mathbf{k}_{\perp} = -\infty$  to  $\mathbf{k}_{\perp} = \infty$ . Far apart from the Fermi surfaces, we can regulate the gap function as  $\hat{\Delta}(\mathbf{k}) \rightarrow 0$  at  $\mathbf{k}_{\perp} = \pm\infty$  and neglect off-diagonal terms in  $\mathcal{E}(\mathbf{k})$  without changing the physics. With this regularization,  $\det \hat{q}(\mathbf{k})$  becomes identical at  $\mathbf{k}_{\perp} = \pm\infty$ . As a result, we can show that the topological number  $W(\mathbf{k}_{\parallel})$  takes an integer value. On the other hand, for lattice models of superconductors, the line integral in (11) should be performed in the noncontractable closed loop  $C$  in the Brillouin zone as illustrated in Fig.2. In this case, the periodicity of the Hamiltonian with respect to a reciprocal vector  $\mathbf{G}$ ,  $\mathcal{H}(\mathbf{k}) = \mathcal{H}(\mathbf{k} + \mathbf{G})$ , ensures the quantization of  $W(\mathbf{k}_{\parallel})$ .

From the bulk-edge correspondence, we obtain the following simple criterion for the ABS<sup>107,108,115,126</sup>:

- *When the topological number  $W(\mathbf{k}_{\parallel})$  takes a non-zero integer, a dispersionless ABS exists on the surface.*

We notice here that the resultant ABS has flat dispersion: This is because the topological number  $W(\mathbf{k}_{\parallel})$  is nonzero in a finite region of  $\mathbf{k}_{\parallel}$  since it cannot change unless the integration

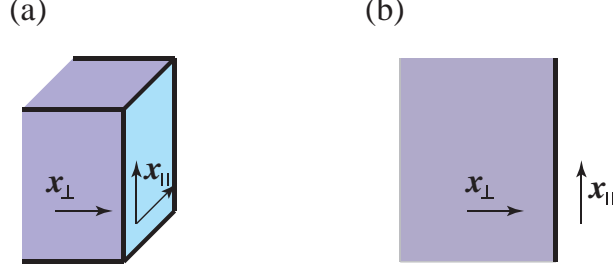


FIG. 1: (color online) Surfaces of superconductors. (a) two dimensional surface. (b) 1 dimensional edge. The conjugate momenta of  $\mathbf{x}_\perp$  and  $\mathbf{x}_\parallel$  are  $\mathbf{k}_\perp$  and  $\mathbf{k}_\parallel$ , respectively.

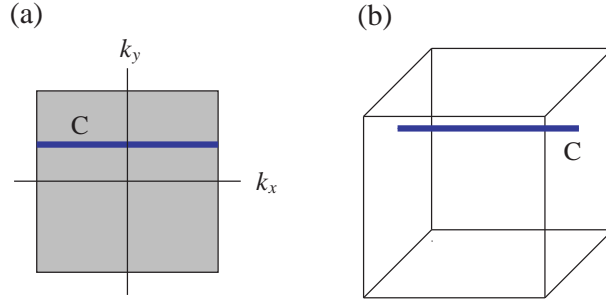


FIG. 2: (color online) The integral path  $C$  in the first Brillouin zone. (a) two dimensional case. (b) three dimensional case. On the path  $C$ , the momentum  $\mathbf{k}$  has a fixed  $\mathbf{k}_\parallel$ .

path intersects a gap node. From the above criterion, this implies that the zero energy ABS also exists in a finite region of  $\mathbf{k}_\parallel$ . In other words, the ABS obtained from the above criterion has flat dispersion. On the other hand, if the integration path intersects a gap node,  $\det \hat{q}(\mathbf{k})$  becomes zero, thus a discontinuous change of  $W(\mathbf{k}_\parallel)$  becomes possible. (Note that at a gap node  $\mathbf{k}_0$ ,  $\det \mathcal{H}(\mathbf{k}_0) \propto |\det \hat{q}(\mathbf{k}_0)|^2 = 0$ .) Therefore, we find that

- *the flat dispersion ABSs are terminated in a gap node in the surface momentum  $\mathbf{k}_\parallel$  space.*

These results are confirmed in concrete examples in Secs.IV and V, and proved eventually in Sec.VI.

### III. CHIRALITY AND TOPOLOGICAL STABILITY OF ANDREEV BOUND STATE

In the previous section, we discussed the topological number constructed from the bulk BdG Hamiltonian  $\mathcal{H}(\mathbf{k})$  which ensures the existence of the dispersionless ABS. In this section, we present an alternative argument on the stability of the flat dispersion ABS from a viewpoint of the boundary. This argument reveals a peculiar spin structure of the dispersionless ABSs, which we call chirality, from which the scattering between them is much suppressed.

In order to argue the boundary state, we perform the Fourier transformation of the BdG Hamiltonian  $\mathcal{H}(\mathbf{k})$  with respect to  $\mathbf{k}_\perp$ , and denote the resultant BdG Hamiltonian as  $\mathcal{H}(\mathbf{x}_\perp, \mathbf{k}_\parallel)$ , where  $\mathbf{x}_\perp$  is the conjugate coordinate of  $\mathbf{k}_\perp$ . Then consider the semi-infinite superconductor on  $\mathbf{x}_\perp > 0$  where the surface is located on  $\mathbf{x}_\perp = 0$ . The corresponding BdG equation is given by

$$\mathcal{H}(\mathbf{x}_\perp, \mathbf{k}_\parallel)|u(\mathbf{x}_\perp, \mathbf{k}_\parallel)\rangle = E(\mathbf{k}_\parallel)|u(\mathbf{x}_\perp, \mathbf{k}_\parallel)\rangle, \quad (12)$$

with the boundary condition

$$|u(\mathbf{x}_\perp, \mathbf{k}_\parallel)\rangle = 0, \quad (13)$$

at  $\mathbf{x}_\perp = 0$ . The zero energy ABS satisfies (12) and (13) with  $E(\mathbf{k}_\parallel) = 0$ .

In our argument, it is convenient to use the following equation

$$\mathcal{H}^2(\mathbf{x}_\perp, \mathbf{k}_\parallel)|v(\mathbf{x}_\perp, \mathbf{k}_\parallel)\rangle = E^2(\mathbf{k}_\parallel)|v(\mathbf{x}_\perp, \mathbf{k}_\parallel)\rangle. \quad (14)$$

instead of the original BdG equation (12). As is shown in Appendix A, it is found that there exists one to one correspondence between the solutions of the BdG equation (12) and those of (14). In particular, the zero energy state  $|u_0(\mathbf{x}_\perp, \mathbf{k}_\parallel)\rangle$  of (12) is exactly the same as the state  $|v_0(\mathbf{x}_\perp, \mathbf{k}_\parallel)\rangle$  of (14) with  $E^2(\mathbf{k}_\parallel) = 0$ . Therefore, we consider (14) instead of (12) in the following.

The starting point of our argument is the chiral symmetry (7) of the BdG Hamiltonian. From (7), we have

$$\{\mathcal{H}(\mathbf{x}_\perp, \mathbf{k}_\parallel), \Gamma\} = 0, \quad (15)$$



thus,  $\mathcal{H}^2(\mathbf{x}_\perp, \mathbf{k}_\parallel)$  and  $\Gamma$  commute with each other,

$$[\mathcal{H}^2(\mathbf{x}_\perp, \mathbf{k}_\parallel), \Gamma] = 0. \quad (16)$$

Therefore, the solution  $|v(\mathbf{x}_\perp, \mathbf{k}_\parallel)\rangle$  of (14) can be an eigenstate of  $\Gamma$  at the same time. Then we denote the solution with the eigenvalue  $\Gamma = \pm 1$  as  $|v^{(\pm)}(\mathbf{x}_\perp, \mathbf{k}_\parallel)\rangle$ . From the argument in Appendix A, we find the following properties of  $|v^{(\pm)}(\mathbf{x}_\perp, \mathbf{k}_\parallel)\rangle$ .

1. For a solution with nonzero  $E^2(\mathbf{k}_\parallel) \neq 0$ , the state  $|v^{(+)}(\mathbf{x}_\perp, \mathbf{k}_\parallel)\rangle$  is always paired with  $|v^{(-)}(\mathbf{x}_\perp, \mathbf{k}_\parallel)\rangle$ . In other words, for nonzero energy solutions, the number of the  $\Gamma = 1$  states is equal to that of the  $\Gamma = -1$  states.
2. On the other hand, for zero energy solutions, the number of the  $\Gamma = 1$  states is not always the same as that of the  $\Gamma = -1$  states.

If we denote the number of the zero energy state with  $\Gamma = \pm 1$  as  $N_0^{(\pm)}$ , these properties imply that  $N_0^{(+)} - N_0^{(-)}$  does not change its value against perturbation preserving the chiral symmetry. As illustrated in Fig.3, some of the zero energy states might acquire non-zero energy by the perturbation, however, they always form a pair with opposite chirality  $\Gamma$ . So the difference  $N_0^{(+)} - N_0^{(-)}$  does not change as a result. This result implies that the existence of the zero energy state is robust against the perturbation once  $N_0^{(+)} - N_0^{(-)}$  becomes nonzero.

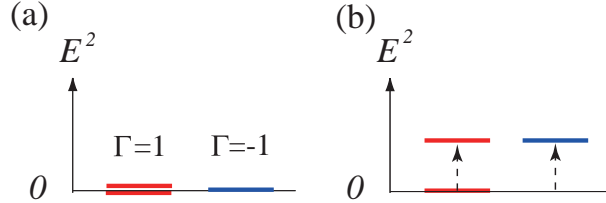


FIG. 3: (color online) Zero energy states of  $\mathcal{H}^2(\mathbf{x}_\perp, \mathbf{k}_\parallel)$ . (a)  $N_0^{(+)} = 2$  and  $N_0^{(-)} = 1$ . (b)  $N_0^{(+)} = 1$  and  $N_0^{(-)} = 0$ . By perturbation, some of the zero modes in (a) might become non-zero modes as in (b), however,  $N_0^{(+)} - N_0^{(-)}$  does not change.

As was shown in the previous section, from the bulk-edge correspondence, we find that the nonzero  $W(\mathbf{k}_\parallel)$  implies the existence of the zero energy ABS. At the same time, in this section, we find that the nonzero  $N_0^{(+)} - N_0^{(-)}$  also ensures the robustness of the existence of the zero energy state. Therefore, it is naturally conjectured that these two quantities,

$W(\mathbf{k}_{\parallel})$  and  $N_0^{(+)} - N_0^{(-)}$ , should be equaled. Since there is a sign ambiguity to equal these two quantities, we have two possible equations in a form of index theorems,

$$W(\mathbf{k}_{\parallel}) = N_0^{(-)} - N_0^{(+)}, \quad (17)$$

or

$$W(\mathbf{k}_{\parallel}) = N_0^{(+)} - N_0^{(-)}. \quad (18)$$

In the following examples, we will show that the conjecture of the index theorem (17) or (18) indeed holds. Then they will be proved eventually in Sec.VI. Here note that there are two possible choices of the surfaces of the superconductor which is perpendicular to  $\mathbf{x}_{\perp}$ , i.e. the surface of the semi-infinite superconductor on  $\mathbf{x}_{\perp} > 0$  or that on  $\mathbf{x}_{\perp} < 0$ . It will be found that these two possible choices of the surface exactly correspond to the two possible equalities (17) and (18).

#### IV. SIGN CHANGE OF GAP FUNCTION AND TOPOLOGICAL CRITERION IN SUPERCONDUCTOR PRESERVING $S_z$ <sup>126</sup>

We first consider the simplest case where the Cooper pair preserves spin in a certain direction, say  $S_z$ . As is shown below, the gap function consists of a real single component, and the BdG Hamiltonian reduces to a  $2 \times 2$  matrix in this case. Since the particle-hole symmetry (6) and the time-reversal invariance (4) have different forms in the  $2 \times 2$  BdG Hamiltonian, it needs a special care to consider this case. In particular, the particle-hole symmetry (6) is not manifest in the  $2 \times 2$  BdG Hamiltonian. Nevertheless, we find a chiral symmetry in the  $2 \times 2$  BdG Hamiltonian in the following, and using it, we will present topological criteria similar to (17) and (18).

In this case, it also has been known that a sign change of the gap function implies the existence of the zero energy ABS.<sup>6,7</sup> Below, we will show that our topological criterion reproduces this result if the Fermi surface has a simple sphere-like shape. In addition, we consider a general Fermi surface, where these two criteria are not coincident with each other. It will be shown that our topological criterion excellently agrees with the details of the zero energy ABS, while the previous one is not.

Let us consider a time-reversal invariant superconductor described by a single-band electron. We also assume that the spin component of a certain direction is preserved. Without

loss of generality, we can select the preserved spin axis as  $z$ , and the gap function is given by

$$\hat{\Delta}(\mathbf{k}) = \begin{cases} i\psi(\mathbf{k})\sigma_y, & \text{for spin-singlet superconductor} \\ id_z(\mathbf{k})\sigma_z\sigma_y, & \text{for spin-triplet superconductor} \end{cases}, \quad (19)$$

where  $\psi(\mathbf{k})$  and  $d_z(\mathbf{k})$  are real functions. Under this assumption, the Hamiltonian  $\mathcal{H}$  reduces to

$$\mathcal{H} = \sum_{\mathbf{k}} \begin{pmatrix} c_{\mathbf{k}\uparrow}^\dagger & c_{-\mathbf{k}\downarrow} \end{pmatrix} \mathcal{H}_{2\times 2}(\mathbf{k}) \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c_{-\mathbf{k}\downarrow}^\dagger \end{pmatrix}, \quad (20)$$

with

$$\mathcal{H}_{2\times 2}(\mathbf{k}) = \begin{pmatrix} \varepsilon(\mathbf{k}) & \Delta(\mathbf{k}) \\ \Delta(\mathbf{k}) & -\varepsilon(\mathbf{k}) \end{pmatrix}. \quad (21)$$

Here  $\Delta(\mathbf{k})$  is given by

$$\Delta(\mathbf{k}) = \begin{cases} \psi(\mathbf{k}) & \text{for spin-singlet superconductor} \\ d_z(\mathbf{k}) & \text{for spin-triplet superconductor} \end{cases}. \quad (22)$$

Note that the BdG Hamiltonian is now reduced to the  $2 \times 2$  matrix (21).

As has been mentioned above, the particle-hole symmetry (6) is not manifest in (21). However, we find the reduced Hamiltonian (21) has the following chiral symmetry,

$$\{\gamma, \mathcal{H}_{2\times 2}(\mathbf{k})\} = 0, \quad \gamma = \sigma_y. \quad (23)$$

Indeed, we can show that the chiral symmetry (23) is indeed a remnant of the original chiral symmetry (7).

In a similar manner as Sec.III, we can define the topological number by using the chiral symmetry (23). By using the unitary transformation  $u_\gamma$  which diagonalizes  $\gamma$  as

$$u_\gamma^\dagger \gamma u_\gamma = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad u_\gamma = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ i & -1 \end{pmatrix}, \quad (24)$$

$\mathcal{H}_{2\times 2}(\mathbf{k})$  is recast into

$$u_\gamma^\dagger \mathcal{H}_{2\times 2}(\mathbf{k}) u_\gamma = \begin{pmatrix} 0 & q(\mathbf{k}) \\ q^*(\mathbf{k}) & 0 \end{pmatrix}, \quad (25)$$

with  $q(\mathbf{k}) = -i\varepsilon(\mathbf{k}) - \Delta(\mathbf{k})$ . Now we introduce the topological number  $w(k_y)$  as

$$\begin{aligned} w(k_y) &= -\frac{1}{4\pi i} \int dk_x \text{tr} [\gamma \mathcal{H}_{2 \times 2}^{-1}(\mathbf{k}) \partial_{k_x} \mathcal{H}_{2 \times 2}(\mathbf{k})] \\ &= \frac{1}{2\pi} \text{Im} \left[ \int dk_x \partial_{k_x} \ln q(\mathbf{k}) \right]. \end{aligned} \quad (26)$$

Here the line integral (26) is performed in a manner similar to (11). As is shown in Appendix B 1, it is found that this integral can be rewritten as the following simple summation,

$$w(k_y) = \frac{1}{2} \sum_{\varepsilon(\mathbf{k})=0} \text{sgn}[\partial_{k_x} \varepsilon(\mathbf{k})] \cdot \text{sgn}[\Delta(\mathbf{k})], \quad (27)$$

where the summation is taken for  $k_x$  satisfying  $\varepsilon(\mathbf{k}) = 0$  with a fixed  $k_y$ . The formula (27) makes it easy to evaluate the topological number  $w(k_y)$ . Then from the bulk-edge correspondence, we can say that if  $w(k_y) \neq 0$ , there exists a dispersionless ABS on a surface of the superconductor which is perpendicular to the  $x$ -direction.

Furthermore, by using an argument similar to that in Sec.III, it is found that the ABS with flat dispersion is an eigenstate of the chirality operator  $\gamma$  again. Then, in a similar manner as (17), we can conjecture that the number  $n_0^{(\pm)}$  of the zero energy ABS with chirality  $\gamma = \pm 1$  satisfies

$$w(k_y) = n_0^{(-)} - n_0^{(+)}, \quad (28)$$

or

$$w(k_y) = n_0^{(+)} - n_0^{(-)}. \quad (29)$$

These give a criterion for the ABS with flat dispersion.

We notice here that our topological criterion of dispersionless ABS includes the criterion proposed previously. In the case where the topology of the Fermi surface is simple as illustrated in Fig.4, it has been known that if the gap function satisfies

$$\Delta(k_x, k_y) \Delta(-k_x, k_y) < 0 \quad (30)$$

then a zero energy ABS exists on the boundary perpendicular to  $x$ -direction.<sup>6,7</sup> In other words, a sign change of the gap function with respect to  $k_x \rightarrow -k_x$  implies the existence of the zero energy ABS on a surface perpendicular to the  $x$ -direction. Our topological criterion reproduces this result correctly: The formula (27) leads to

$$w(k_y) = \frac{1}{2} [\text{sgn}[\partial_{k_x} \varepsilon(-k_x^0, k_y)] \cdot \text{sgn}[\Delta(-k_x^0, k_y)] + \text{sgn}[\partial_{k_x} \varepsilon(k_x^0, k_y)] \cdot \text{sgn}[\Delta(k_x^0, k_y)]] \quad (31)$$

where  $(\pm k_x^0, k_y)$  denote the intersection points between the integral path of  $w(k_y)$  and the Fermi surface. See Fig. 4. Noticing that  $\text{sgn}[\partial_{k_x}\varepsilon(k_x^0, k_y)] = -\text{sgn}[\partial_{k_x}\varepsilon(-k_x^0, k_y)]$ , we can rewrite this as

$$w(k_y) = \frac{1}{2}\text{sgn}[\partial_{k_x}\varepsilon(-k_x^0, k_y)] [\text{sgn}[\Delta(-k_x^0, k_y)] - \text{sgn}[\Delta(k_x^0, k_y)]] . \quad (32)$$

Thus the topological number  $w(k_y)$  becomes nonzero only when the gap function satisfies (30), which means that our topological criterion reproduces the previous one in this particular simple case.

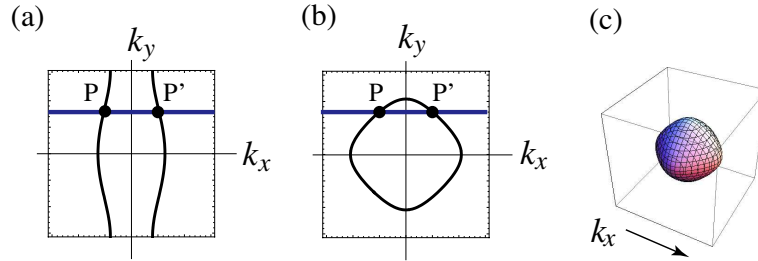


FIG. 4: (color online) Fermi surfaces with simple topology in (a) quasi-one dimensional system, (b) quasi-two dimensional one, and (c) three dimensional one. The thick blue lines denote the integral path of  $w$ . For simplicity, we illustrate the integral path only in (a) and (b). For each case, the integral path gets across the Fermi surface only twice at  $k_x = \pm k_x^0$ . In (a) and (b), P and P' denote the intersection point  $(-k_x^0, k_y)$  and  $(k_x^0, k_y)$ , respectively.

We would like to emphasize here that our topological criterion does not merely reproduce the known criterion, but is more informative. First, the chirality of the zero energy ABS is determined in a manner consistent with the formulas (28) and (29). Second, our formula is also applicable to more complicated cases in which the previous criterion does not work. We will see them in Secs. IV A, IV B and IV D.

#### A. $d_{xy}$ -wave superconductor

Here we consider the  $d_{xy}$ -wave superconductor where  $\varepsilon(\mathbf{k})$  and  $\Delta(\mathbf{k})$  in (21) are given by

$$\varepsilon(\mathbf{k}) = \frac{\mathbf{k}^2}{2m} - \mu, \quad \Delta(\mathbf{k}) = \Delta_0 \frac{k_x k_y}{k^2}. \quad (33)$$

Here  $\Delta_0$  is a positive constant. From (27), the topological number  $w(k_y)$  is evaluated as

$$w(k_y) = \begin{cases} 1, & \text{for } 0 < k_y < k_F \\ -1, & \text{for } 0 > k_y > -k_F \\ 0, & \text{for } |k_y| > k_F \end{cases}, \quad (34)$$

where  $k_F = \sqrt{2m\mu}$  is the Fermi momentum. Thus our topological criterion (28) implies the existence of the zero energy ABS for  $|k_y| < k_F$ .

Now, let us solve the BdG equation for the semi-infinite  $d_{xy}$  superconductor on  $x > 0$  with the boundary condition  $|u(x=0, k_y)\rangle = 0$ . For  $|k_y| < k_F$ , the following zero energy ABS on  $x = 0$  is found<sup>6</sup>

$$|u_0(x)\rangle = C \begin{pmatrix} 1 \\ -i\text{sgn}k_y \end{pmatrix} e^{ik_y y} \sin(k_x x) e^{-x/\xi}, \quad (35)$$

where  $C$  is a normalization constant,  $k_x = \sqrt{k_F^2 - k_y^2}$  and  $\xi^{-1} = m\Delta_0 k_y / k_F^2$ . Since the ABS is an eigenstate of  $\gamma (= \sigma_y)$  with eigenvalue  $\gamma = -1$  ( $\gamma = 1$ ) for  $0 < k_y < k_F$  ( $0 > k_y > -k_F$ ), it is found that  $n_0^{(+)} = 0$  and  $n_0^{(-)} = 1$  for  $0 < k_y < k_F$  ( $n_0^{(+)} = 1$  and  $n_0^{(-)} = 0$  for  $0 > k_y > -k_F$ ). On the other hand, for  $|k_y| > k_F$ , we do not find any zero energy ABS, thus  $n_0^{(+)} = n_0^{(-)} = 0$ . We summarize these results in Table I (a), which shows that the index theorem (28) holds in this case.

If we choose the semi-infinite  $d_{xy}$  superconductor on  $x < 0$ , the zero energy ABS on the surface at  $x = 0$  is given by

$$|u_0(x)\rangle = C \begin{pmatrix} 1 \\ i\text{sgn}k_y \end{pmatrix} e^{ik_y y} \sin(k_x x) e^{x/\xi}. \quad (36)$$

Thus  $n_0^{(+)}$  and  $n_0^{(-)}$  are summarized as Table I (b). The index theorem (29) holds in this case.

## B. $p_x$ -wave superconductor

Now consider the semi-infinite  $p_x$ -wave superconductor on  $x > 0$ . The gap function is  $\Delta(\mathbf{k}) = \Delta_0 k_x / k$  with  $k = \sqrt{\mathbf{k}^2}$  and  $\varepsilon(\mathbf{k})$  is the same as that in (33). For the  $p_x$ -wave superconductor, we have

$$w(k_y) = \begin{cases} 1, & \text{for } |k_y| < k_F \\ 0, & \text{for } |k_y| > k_F \end{cases}, \quad (37)$$

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(a)  $d_{xy}$ -wave superconductor on  $x > 0$

$k_y$	$n_0^{(+)}$	$n_0^{(-)}$	$n_0^{(+)} - n_0^{(-)}$	$w(k_y)$
$0 < k_y < k_F$	0	1	-1	1
$0 > k_y > -k_F$	1	0	1	-1
$ k_y  > k_F$	0	0	0	0

(b)  $d_{xy}$ -wave superconductor on  $x < 0$

$k_y$	$n_0^{(+)}$	$n_0^{(-)}$	$n_0^{(+)} - n_0^{(-)}$	$w(k_y)$
$0 < k_y < k_F$	1	0	1	1
$0 > k_y > -k_F$	0	1	-1	-1
$ k_y  > k_F$	0	0	0	0

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TABLE I: The number  $n_0^{(\pm)}$  of the zero energy ABSs with the chirality  $\gamma = \pm 1$  for (a) the semi-infinite  $d_{xy}$ -wave superconductor on  $x > 0$  and (b) that on  $x < 0$ . For comparison, we also show the topological number  $w(k_y)$  given in (34). The index theorem (28) and (29) hold in (a) and (b), respectively.

from (27). Correspondingly, if  $|k_y| < k_F$ , we obtain the following zero energy ABS on  $x = 0$

$$|u(x, k_y)\rangle = \begin{pmatrix} 1 \\ -i \end{pmatrix} e^{ik_y y} \sin(k_x x) e^{-x/\xi_p}, \quad (38)$$

for the semi-infinite  $p_x$ -wave superconductor on  $x > 0$ , and

$$|u(x, k_y)\rangle = \begin{pmatrix} 1 \\ i \end{pmatrix} e^{ik_y y} \sin(k_x x) e^{x/\xi_p}, \quad (39)$$

for the semi-infinite  $p_x$ -wave superconductor on  $x < 0$ . Here  $k_x = \sqrt{k_F^2 - k_y^2}$  and  $\xi_p^{-1} = m\Delta_0/k_F$ . It is also found that these solutions are the eigenstates of  $\gamma$  with the eigenvalue  $\gamma = -1$  and  $\gamma = 1$ , respectively. Thus  $n_0^{(+)}$  and  $n_0^{(-)}$  are summarized as Table II (a) and (b). We confirm the relations (28) and (29), respectively again.

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(a)  $p_x$ -wave superconductor on  $x > 0$

$k_y$	$n_0^{(+)}$	$n_0^{(-)}$	$n_0^{(+)} - n_0^{(-)}$	$w(k_y)$
$ k_y  < k_F$	0	1	-1	1
$ k_y  > k_F$	0	0	0	0

(b)  $p_x$ -wave superconductor on  $x < 0$

$k_y$	$n_0^{(+)}$	$n_0^{(-)}$	$n_0^{(+)} - n_0^{(-)}$	$w(k_y)$
$ k_y  < k_F$	1	0	1	1
$ k_y  > k_F$	0	0	0	0

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TABLE II: The number  $n_0^{(\pm)}$  of the zero energy ABSs with the chirality  $\gamma = \pm 1$  for (a) the semi-infinite  $p_x$ -wave superconductor on  $x > 0$  and (b) that on  $x < 0$ , respectively. For comparison, we also show the topological number  $w(k_y)$  given in (37). The index theorem (28) and (29) hold in (a) and (b), respectively.

### C. Zero energy Andreev bound state and odd-frequency pairing

In this subsection, we discuss the ABS in  $d_{xy}$ -wave and  $p_x$ -wave superconductors from a viewpoint of odd-frequency pairing. It will be shown that the odd-frequency pairing has a topological structure similar to that of the ABSs discussed in Secs. IV A and IV B.

Odd-frequency pairing is the pair function (pairing amplitude) that changes a sign when exchanging the time coordinates of two electrons.<sup>127</sup> Thus the Fourier transformed pairing function is an odd function of frequency. Near the surface of superconductor, due to the breakdown of translational invariance, the pair potential acquires a spatial dependence leading to the coupling between the even and odd-parity pairing states. From the Fermi-Dirac statistics, the induced pair amplitude at the interface should be odd in frequency. It has been established recently that zero energy dispersionless ABSs induce odd-frequency pairings at the surface of the superconductors.<sup>49–52</sup>

First, we consider a two-dimensional semi-infinite superconductor in  $x > 0$  where the surface is located at  $x = 0$ . As shown in the appendix D, the pair amplitude at the surface



of  $d_{xy}$ -wave superconductor is given by

$$f(k_x, k_y) = \frac{i \text{sgn}(k_y) \Delta_0}{\omega_n} \frac{|k_x| |k_y|}{\mathbf{k}^2} \quad (40)$$

in the Matsubara representation. Thus the odd-parity odd-frequency pairing is realized at the surface. On the other hand, for  $p_x$ -wave pair potential, we obtain

$$f(k_x, k_y) = \frac{i \Delta_0}{\omega_n} \frac{|k_x|}{\sqrt{\mathbf{k}^2}}, \quad (41)$$

which means the realization of even-parity odd-frequency pairing in this case. As well as the wave function of zero energy ABS of  $d_{xy}$  and  $p_x$ -wave superconductor in Secs. IV A and IV B, the factor  $\text{sgn} k_y$  exists only for  $d_{xy}$ -wave case. This factor decides the difference of the parity of induced Cooper pair. The difference of the parity results in a serious difference when we consider proximity effect into DN attached to superconductor<sup>49,51,52</sup>. In DN, only  $s$ -wave even parity pairing is possible. Thus, odd-parity odd-frequency pairing amplitude cannot penetrate into DN. This implies that ABS in  $d_{xy}$ -wave superconductor cannot enter into DN since it is expressed by odd-frequency spin-singlet odd-parity state. On the other hand, for  $p_x$ -wave superconductor, ABS can enter into DN since it is expressed by odd-frequency spin-singlet even-parity state including  $s$ -wave channel<sup>44–48</sup>.

Now we consider a two-dimensional semi-infinite superconductor in  $x < 0$ . The corresponding pair amplitude at surface ( $x = 0$ ) is given by

$$f(k_x, k_y) = -\frac{i \text{sgn}(k_y) \Delta_0}{\omega_n} \frac{|k_x| |k_y|}{\mathbf{k}^2} \quad (42)$$

for spin-singlet  $d_{xy}$ -wave superconductor and

$$f(k_x, k_y) = -\frac{i \Delta_0}{\omega_n} \frac{|k_x|}{\sqrt{\mathbf{k}^2}} \quad (43)$$

for spin-triplet  $p_x$ -wave one, respectively. Comparing Eq. (40) [(41)] with (42) [(43)], we find the difference between them is the presence of  $-\text{sign}$ . The present  $-\text{sign}$  exactly corresponds to the different values of  $n_0^+$  and  $n_0^-$  between case (a) and case (b) in Tables I and II.

#### D. Dispersionless Andreev bound states in superconductors with multiple Fermi surfaces

In the above two examples, we assume a simple Fermi surface obtained in (33). Here we consider superconducting states with more complicated Fermi surfaces. To realize multiple

Fermi surfaces, we consider a model in the square lattice. By taking into account the second next nearest-neighbor hopping, the normal dispersion  $\varepsilon(\mathbf{k})$  is given by

$$\varepsilon(\mathbf{k}) = -2t[\cos k_x + \cos k_y] - 2t'[\cos 2k_x + \cos 2k_y] - \mu. \quad (44)$$

As illustrated in Fig.5, if we choose the parameters  $t$ ,  $t'$  and  $\mu$  properly, multiple Fermi surfaces are realized in the first Brillouin zone.

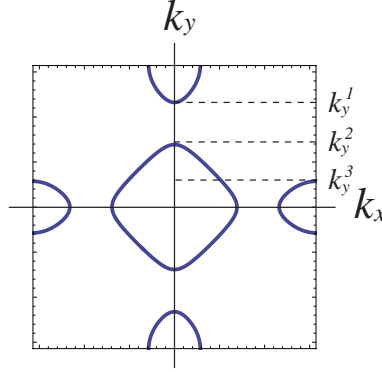


FIG. 5: (color online) The multiple Fermi surfaces in the first Brillouin zone. We take  $t = t' = 1$  and  $\mu = -2.5$  in (44).

For the gap function, we consider (a)  $d_{xy}$ -wave pairing with  $\Delta(\mathbf{k}) = \Delta_0 \sin k_x \sin k_y$ , (b)  $p_x$ -wave pairing with  $\Delta(\mathbf{k}) = \Delta_0 \sin k_x$  and (c)  $p_x$ -wave pairing with  $\Delta(\mathbf{k}) = \Delta_0 \sin 2k_x$ . Since the condition (30) is satisfied in all the cases in the above, the sign change criterion suggests the existence of zero energy ABS on a surface perpendicular to the  $x$ -direction. However, we find that zero energy ABSs do not always appear.

To study the edge state, we consider the model above in the square lattice. The BdG Hamiltonian in the lattice space is given by

$$\begin{aligned} \mathcal{H} &= \mathcal{H}_{\text{kin}} + \mathcal{H}_s, \\ \mathcal{H}_{\text{kin}} &= -t \sum_{\langle \mathbf{i}, \mathbf{j} \rangle, \sigma} c_{\mathbf{i}, \sigma}^\dagger c_{\mathbf{j}, \sigma} - t' \sum_{\langle\langle \mathbf{i}, \mathbf{j} \rangle\rangle, \sigma} c_{\mathbf{i}, \sigma}^\dagger c_{\mathbf{j}, \sigma} - \mu \sum_{\mathbf{i}, \sigma} c_{\mathbf{i}, \sigma}^\dagger c_{\mathbf{i}, \sigma}, \end{aligned} \quad (45)$$

where  $\mathbf{i} = (i_x, i_y)$  denotes a site on the square lattice,  $c_{\mathbf{i}, \sigma}^\dagger$  ( $c_{\mathbf{i}, \sigma}$ ) the creation (annihilation) operator of an electron with spin  $\sigma$  at site  $\mathbf{i}$ . The summation  $\langle \mathbf{i}, \mathbf{j} \rangle$  ( $\langle\langle \mathbf{i}, \mathbf{j} \rangle\rangle$ ) is taken for the nearest-neighbor (the second next nearest-neighbor) sites.  $\mathcal{H}_s$  is the pairing term depending

on the symmetry of the Cooper pair. For the  $d_{xy}$ -wave pairing with  $\Delta(\mathbf{k}) = \Delta_0 \sin k_x \sin k_y$ , it is given by

$$\mathcal{H}_s = -\frac{\Delta_0}{4} \sum_{\mathbf{i}} (c_{\mathbf{i}+\hat{x}+\hat{y},\uparrow}^\dagger c_{\mathbf{i},\downarrow}^\dagger + c_{\mathbf{i}-\hat{x}-\hat{y},\uparrow}^\dagger c_{\mathbf{i},\downarrow}^\dagger - c_{\mathbf{i}+\hat{x}-\hat{y},\uparrow}^\dagger c_{\mathbf{i},\downarrow}^\dagger - c_{\mathbf{i}-\hat{x}+\hat{y},\uparrow}^\dagger c_{\mathbf{i},\downarrow}^\dagger) + \text{h.c.} \quad (46)$$

For the  $p_x$ -wave pairing with  $\Delta(\mathbf{k}) = \Delta_0 \sin k_x$ ,

$$\mathcal{H}_s = \frac{\Delta_0}{2i} \sum_{\mathbf{i}} (c_{\mathbf{i},\uparrow}^\dagger c_{\mathbf{i}+\hat{x},\downarrow}^\dagger - c_{\mathbf{i},\uparrow}^\dagger c_{\mathbf{i}-\hat{x},\downarrow}^\dagger) + \text{h.c.}, \quad (47)$$

and for the  $p_x$ -wave pairing with  $\Delta(\mathbf{k}) = \Delta_0 \sin 2k_x$ ,

$$\mathcal{H}_s = \frac{\Delta_0}{2i} \sum_{\mathbf{i}} (c_{\mathbf{i},\uparrow}^\dagger c_{\mathbf{i}+2\hat{x},\downarrow}^\dagger - c_{\mathbf{i},\uparrow}^\dagger c_{\mathbf{i}-2\hat{x},\downarrow}^\dagger) + \text{h.c.} \quad (48)$$

Suppose that the system has two open boundary edges at  $i_x = 0$  and  $i_x = N_x$ , and impose the periodic boundary condition in the  $y$ -direction. Solving numerically the energy spectrum as a function of the momentum  $k_y$ , we examine the edge states.

In Fig.6(a)-(c), we illustrate the energy spectra for each case. In spite that zero energy ABSs appear on the edges, the previous criterion does not explain the detailed structures. Indeed, in the cases (a) and (b), the dispersionless ABSs disappear near  $k_y \sim 0$ , although the sign change condition (30) is still satisfied for both cases. Therefore, the sign change criterion does not work in these cases. On the other hand, the topological criterion does work in all the cases. From the formula (27), we obtain  $w(k_y)$  in Table III. Comparing  $w(k_y)$  in Table III with the zero energy states in Fig. 6, we find an excellent agreement between them. In particular, for (a) and (b), we find that  $w(k_y) = 0$  at  $k_y \sim 0$  (i.e.  $k_y^3 > k_y > -k_y^3$ ). Thus in contrast to the sign change criterion, our topological criterion explains the detailed structures of the dispersionless ABSs.

## V. NONCENTROSYMMETRIC SUPERCONDUCTOR

In this section, we apply our topological criterion to time-reversal invariant superconductors supporting multiple components of the gap function. For simplicity, we consider the superconductor in a single-band description. In a single-band description, the general BdG Hamiltonian for time-reversal invariant superconductor is given by

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} \varepsilon(\mathbf{k}) + \mathbf{g}(\mathbf{k}) \cdot \boldsymbol{\sigma} & \hat{\Delta}(\mathbf{k}) \\ \hat{\Delta}^\dagger(\mathbf{k}) & -\varepsilon(\mathbf{k}) + \mathbf{g}(\mathbf{k}) \cdot \boldsymbol{\sigma}^* \end{pmatrix}, \quad (49)$$

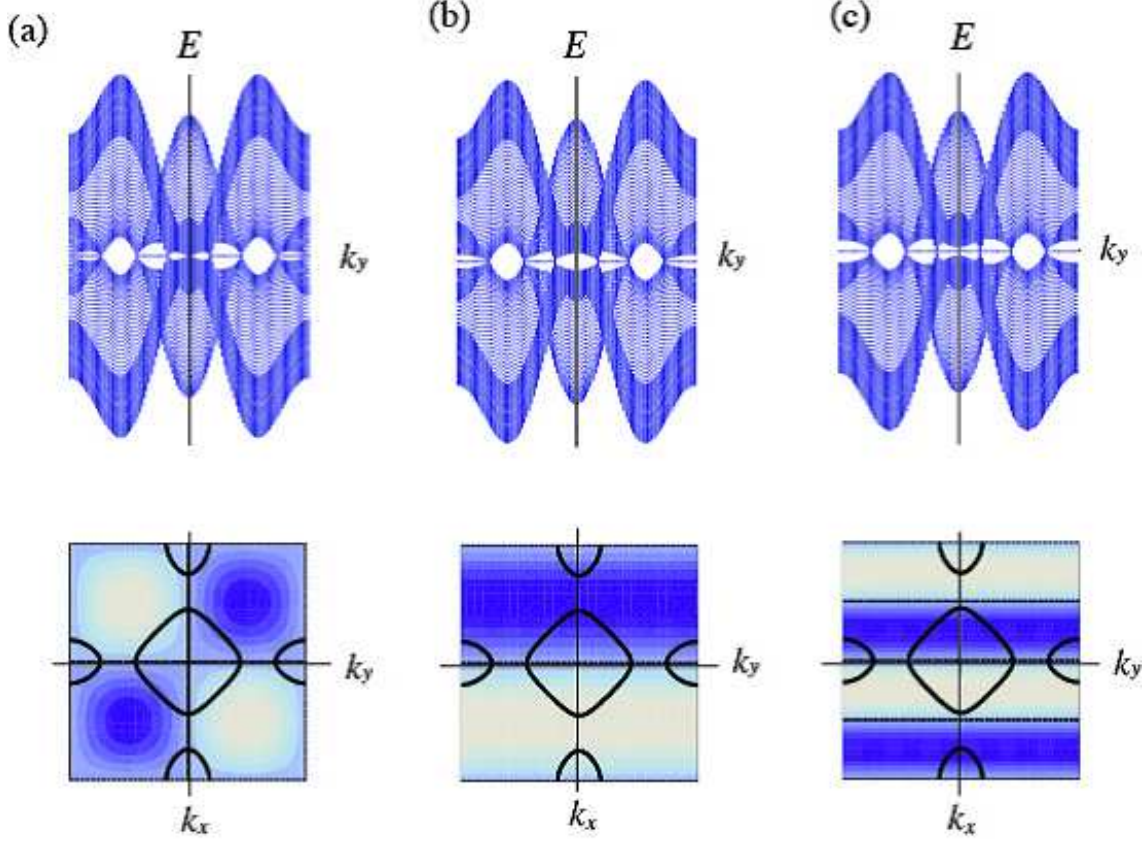


FIG. 6: (color online) The energy spectra with open edges at  $i_x = 0$  and  $i_x = 100$  (upper panels) and the corresponding gap functions in the first Brillouin zone (lower panels) for superconductors with multiple Fermi surfaces. (a)  $d_{xy}$ -wave superconductor with  $\Delta(\mathbf{k}) = \Delta_0 \sin k_x \sin k_y$ , (b)  $p_x$ -wave superconductor with  $\Delta(\mathbf{k}) = \Delta_0 \sin k_x$ , and (c)  $p_x$ -wave superconductor with  $\Delta(\mathbf{k}) = \Delta_0 \sin 2k_x$ . We take  $t = t' = 1$  and  $\mu = -2.5$ .  $\Delta_0$  is chosen as  $\Delta_0 = 1$  for (a) and  $\Delta_0 = 0.5$  for (b) and (c), respectively. In the upper panels,  $k_y$  is the momentum in the  $y$ -direction, and  $k_y \in [-\pi, \pi]$ . The ABSs appear as zero energy states with flat dispersion. In the lower panels, the solid curves denotes the Fermi surfaces. The darker areas denotes the negative gap functions, the lighter areas the positive ones, and the gap functions vanish at the dashed lines. As a matter of convenience, we take the horizontal axis as the  $k_y$ -direction in the lower panels.

where  $\varepsilon(\mathbf{k}) = \varepsilon(-\mathbf{k})$  is the kinetic energy of electron measured from the Fermi energy,  $\mathbf{g}(\mathbf{k}) = -\mathbf{g}(-\mathbf{k})$  the anti-symmetric spin-orbit interaction such as the Rashba spin-orbit coupling,  $\hat{\Delta}(\mathbf{k})$  the gap function  $\hat{\Delta}(\mathbf{k}) = i\psi(\mathbf{k})\sigma_y + i\mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\sigma}\sigma_y$ . This Hamiltonian has the particle-hole symmetry (6) and the time-reversal invariance (4) with  $U = i\sigma_y$ . Thus it also

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$k_y$	$w(k_y)$		
	(a)	(b)	(c)
$\pi > k_y > k_y^1$	1	1	1
$k_y^1 > k_y > k_y^2$	0	0	0
$k_y^2 > k_y > k_y^3$	1	1	1
$k_y^3 > k_y > -k_y^3$	0	0	2
$-k_y^3 > k_y > -k_y^2$	-1	1	1
$-k_y^2 > k_y > -k_y^1$	0	0	0
$-k_y^1 > k_y > -\pi$	-1	1	1

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TABLE III: Topological number  $w(k_y)$  for (a) the  $d_{xy}$ -wave superconductor with  $\Delta(\mathbf{k}) = \Delta_0 \sin k_x \sin k_y$ , and the  $p_x$ -wave superconductor with (b)  $\Delta(\mathbf{k}) = \Delta_0 \sin k_x$  and (c)  $\Delta(\mathbf{k}) = \Delta_0 \sin 2k_x$ . We suppose that  $t = t' = 1$ ,  $\mu = -2.5$  and  $\Delta_0 > 0$ . Here  $k_y^i$  ( $i = 1, 2, 3$ ) are defined in Fig.5.

satisfies (7) with

$$\Gamma = \begin{pmatrix} 0 & \sigma_y \\ \sigma_y & 0 \end{pmatrix}. \quad (50)$$

For the dispersionless ABS for the semi-infinite superconductor on  $x > 0$ , the topological number (11) is given by

$$W(k_y) = \frac{1}{2\pi} \text{Im} \left[ \int dk_x \partial_{k_x} \ln \det \hat{q}(\mathbf{k}) \right], \quad (51)$$

with  $\hat{q}(\mathbf{k}) = [\varepsilon(\mathbf{k}) - i\psi(\mathbf{k})]\sigma_y + [\mathbf{g}(\mathbf{k}) - i\mathbf{d}(\mathbf{k})] \cdot \boldsymbol{\sigma} \sigma_y$ . As is shown in Appendix B2,  $W(k_y)$  is evaluated as

$$W(k_y) = -\frac{1}{2} \sum_{\varepsilon(\mathbf{k})^2 - \mathbf{g}(\mathbf{k})^2 = 0} \text{sgn} [\mathbf{g}(\mathbf{k}) \cdot \mathbf{d}(\mathbf{k}) - \varepsilon(\mathbf{k})\psi(\mathbf{k})] \cdot \text{sgn} [\partial_{k_x} (\varepsilon(\mathbf{k})^2 - \mathbf{g}(\mathbf{k})^2)], \quad (52)$$

where the summation is taken for  $k_x$  satisfying  $\varepsilon(\mathbf{k})^2 - \mathbf{g}(\mathbf{k})^2 = 0$  with a fixed  $k_y$ .

### A. two-dimensional Rashba superconductor

Now consider two-dimensional Rashba noncentrosymmetric superconductors. Here  $\varepsilon(\mathbf{k})$  is given by (33) and  $\mathbf{g}(\mathbf{k}) = \lambda(\hat{\mathbf{x}}k_y - \hat{\mathbf{y}}k_x)$  where  $\lambda$  is the coupling constant of Rashba spin-orbit interaction. Due to the Rashba spin-orbit interaction, the Fermi surface is split into two as illustrated in Fig.7. The Fermi momenta for the smaller and larger Fermi surface are given by

$$k_1 = -m\lambda + \sqrt{(m\lambda)^2 + 2m\mu}, \quad (53)$$

$$k_2 = m\lambda + \sqrt{(m\lambda)^2 + 2m\mu}, \quad (54)$$

respectively. The spin-orbit interaction also mixes the parity of the gap function generally, so the spin-singlet component and the spin-triplet one coexist in the gap function<sup>93,128,129</sup>. The spin-triplet component  $\mathbf{d}(\mathbf{k})$  is aligned with the polarization vector of the Rashba spin orbit coupling,  $\mathbf{d}(\mathbf{k}) \parallel \mathbf{g}(\mathbf{k})$ <sup>93</sup>. Then, the triplet component is given by

$$\mathbf{d}(\mathbf{k}) = \Delta_t f(\mathbf{k})(\hat{\mathbf{x}}k_y - \hat{\mathbf{y}}k_x)/k \quad (55)$$

with  $k = \sqrt{\mathbf{k}^2}$  while the singlet component reads

$$\psi(\mathbf{k}) = \Delta_s f(\mathbf{k}) \quad (56)$$

with  $\Delta_t \geq 0$  and  $\Delta_s \geq 0$ . The superconducting gaps are  $\Delta_1 = |\bar{\Delta}_1(\mathbf{k})|$  and  $\Delta_2 = |\bar{\Delta}_2(\mathbf{k})|$  for the two spin split bands with  $\bar{\Delta}_1(\mathbf{k}) = (\Delta_t + \Delta_s)f(\mathbf{k})$  and  $\bar{\Delta}_2(\mathbf{k}) = (\Delta_t - \Delta_s)f(\mathbf{k})$ .

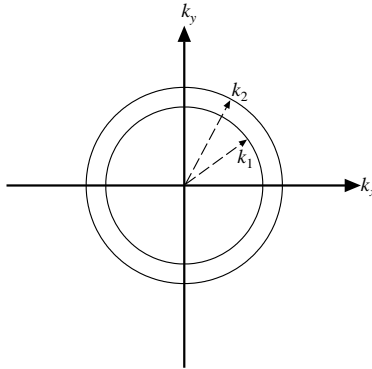


FIG. 7: (color online) Fermi surfaces of two-dimensional Rashba noncentrosymmetric SC.

Using the formula (52), we evaluate the topological number  $W(k_y)$ . We obtain

$$W(k_y) = \frac{1}{2}\text{sgn}[(\Delta_t - \Delta_s)f(-\mathbf{k}_2)] - \frac{1}{2}\text{sgn}[(\Delta_t - \Delta_s)f(\mathbf{k}_2)] \\ - \frac{1}{2}\text{sgn}[(\Delta_t + \Delta_s)f(-\mathbf{k}_1)] + \frac{1}{2}\text{sgn}[(\Delta_t + \Delta_s)f(\mathbf{k}_1)] \quad (57)$$

for  $|k_y| < k_1$ ,

$$W(k_y) = \frac{1}{2}\text{sgn}[(\Delta_t - \Delta_s)f(-\mathbf{k}_2)] - \frac{1}{2}\text{sgn}[(\Delta_t - \Delta_s)f(\mathbf{k}_2)] \quad (58)$$

for  $k_1 < |k_y| < k_2$ , and  $W(k_y) = 0$  for  $k_2 < |k_y|$ . Here,  $\pm\mathbf{k}_i = (\pm\sqrt{k_i^2 - k_y^2}, k_y)$  ( $i = 1, 2$ ).

From Eqs.(57) and (58), it is found that  $W(k_y)$  is nonzero only when  $f(\mathbf{k})$  is an odd function with respect to  $k_x$ . Therefore, for example, for an  $s + p$ -wave or a  $d_{x^2-y^2} + f$ -wave Rashba superconductor, where  $f(\mathbf{k})$  is given by  $f(\mathbf{k}) = 1$  or  $f(\mathbf{k}) = (k_x^2 - k_y^2)/\mathbf{k}^2$ , respectively,  $W(k_y)$  becomes zero. Consistently, we find that they do not support the dispersionless ABSs. On the other hand, for a  $d_{xy} + p$ -wave superconductor, we have a dispersionless ABS.

#### 1. $d_{xy} + p$ -wave superconductor

For the  $d_{xy} + p$ -wave superconductor, we have  $f(\mathbf{k}) = k_x k_y / \mathbf{k}^2$ . Thus,  $W(k_y)$  can be nonzero value. From Eqs. (57) and (58), we obtain

$$W(k_y) = \begin{cases} 2\text{sgn}k_y, & \text{for } |k_y| < k_1 \\ \text{sgn}k_y, & \text{for } k_1 < |k_y| < k_2 \\ 0, & \text{for } |k_y| > k_2 \end{cases} \quad (59)$$

for  $\Delta_s > \Delta_t$ , and

$$W(k_y) = \begin{cases} 0, & \text{for } |k_y| < k_1 \\ -\text{sgn}k_y, & \text{for } k_1 < |k_y| < k_2 \\ 0, & \text{for } |k_y| > k_2 \end{cases} \quad (60)$$

for  $\Delta_t > \Delta_s$ .

To confirm the relation (17), let us consider the two-dimensional semi-infinite  $d_{xy} + p$ -wave Rashba superconductor on  $x > 0$  where the surface is located at  $x = 0$ . The corresponding wave function is given by<sup>98,107</sup>

$$|u(x, k_y)\rangle = [c_1^+ \psi_1^+ \exp(iq_{1x}^+ x) + c_1^- \psi_1^- \exp(-iq_{1x}^- x) + c_2^+ \psi_2^+ \exp(iq_{2x}^+ x) + c_2^- \psi_2^- \exp(-iq_{2x}^- x)] \\ \times \exp(ik_y y), \quad (61)$$

$$q_{1(2)x}^{\pm} = k_{1(2)x}^{\pm} \pm \frac{k_{1(2)}}{k_{1(2)x}^{\pm}} \sqrt{\frac{E^2 - [\bar{\Delta}_{1(2)}(\mathbf{k}_{1(2)}^{\pm})]^2}{\lambda^2 + 2\mu/m}}, \quad (62)$$

with  $k_{1(2)x}^+ = k_{1(2)x}^- = \sqrt{k_{1(2)}^2 - k_y^2}$  for  $|k_y| \leq k_{1(2)}$  and  $k_{1(2)x}^+ = -k_{1(2)x}^- = i\sqrt{k_y^2 - k_{1(2)}^2}$  for  $|k_y| > k_{1(2)}$ , and  $\mathbf{k}_{1(2)}^{\pm} = (\pm k_{1(2)x}^{\pm}, k_y)$ . Here  $\psi_i^{\pm}$  ( $i = 1, 2$ ) are given by

$${}^T\psi_1^{\pm} = (1, -i\alpha_{1\pm}^{-1}, i\alpha_{1\pm}^{-1}\Gamma_{1\pm}, \Gamma_{1\pm}), \quad (63)$$

$${}^T\psi_2^{\pm} = (1, i\alpha_{2\pm}^{-1}, i\alpha_{2\pm}^{-1}\Gamma_{2\pm}, -\Gamma_{2\pm}) \quad (64)$$

with

$$\Gamma_{1(2)\pm} = \frac{\bar{\Delta}_{1(2)}(\mathbf{k}_{1(2)}^{\pm})}{E \pm \sqrt{E^2 - [\bar{\Delta}_{1(2)}(\mathbf{k}_{1(2)}^{\pm})]^2}}, \quad (65)$$

and  $\alpha_{1(2)\pm} = (\pm k_{1(2)x}^{\pm} - ik_y)/k_{1(2)}$ .  $E$  is the quasiparticle energy measured from the Fermi energy. For  $E^2 < [\bar{\Delta}_{1(2)}(\mathbf{k}_{1(2)}^{\pm})]^2$ , the branch of the square root in Eqs.(62) and (65) is chosen so as the wave function (61) is normalized (i.e.  $|u(x, k_y)\rangle \rightarrow 0$  as  $x \rightarrow \infty$ ). When  $E = 0$ , we find

$$\Gamma_{1\pm} = \begin{cases} -i\text{sgn}k_y, & \text{for } |k_y| < k_1 \\ \pm i\text{sgn}k_y, & \text{for } |k_y| > k_1 \end{cases}, \quad (66)$$

and

$$\Gamma_{2\pm} = \begin{cases} -i\text{sgn}(\Delta_t - \Delta_s)\text{sgn}k_y, & \text{for } |k_y| < k_2 \\ \pm i\text{sgn}(\Delta_t - \Delta_s)\text{sgn}k_y, & \text{for } |k_y| > k_2 \end{cases}. \quad (67)$$

Thus, it is found that  $\psi_{1\pm}$  and  $\psi_{2\pm}$  are eigenstates of  $\Gamma$  in (50),

$$\Gamma\psi_1^{\pm} = \begin{cases} -\text{sgn}k_y\psi_1^{\pm}, & \text{for } |k_y| < k_1 \\ \pm\text{sgn}k_y\psi_1^{\pm}, & \text{for } |k_y| > k_1 \end{cases}, \quad (68)$$

$$\Gamma\psi_2^{\pm} = \begin{cases} \text{sgn}(\Delta_t - \Delta_s)\text{sgn}k_y\psi_2^{\pm}, & \text{for } |k_y| < k_2 \\ \mp\text{sgn}(\Delta_t - \Delta_s)\text{sgn}k_y\psi_2^{\pm}, & \text{for } |k_y| > k_2 \end{cases}. \quad (69)$$

In Table IV, we summarize the chirality of  $\psi_{1(2)}^{\pm}$ .

To construct the dispersionless ABS, we put the boundary condition (13) on the wave function above. Then, we have

$$c_1^+\psi_1^+ + c_1^-\psi_1^- + c_2^+\psi_2^+ + c_2^-\psi_2^- = 0. \quad (70)$$



The dispersionless ABS is obtained if there exist non-zero  $c_i^\pm$ s satisfying (70). Applying the chiral projection operator  $P_\pm = (1 \pm \Gamma)/2$  on the both side, we can divide (70) into the sector with  $\Gamma = 1$  and that with  $\Gamma = -1$ . For example, when  $\Delta_s > \Delta_t$  and  $k_2 > k_y > k_1$ , we obtain

$$c_1^+ \psi_1^+ = 0 \quad (71)$$

in the  $\Gamma = 1$  sector, and

$$c_1^- \psi_1^- + c_2^+ \psi_2^+ + c_2^- \psi_2^- = 0, \quad (72)$$

in the  $\Gamma = -1$  sector. Then, we solve (70) in each chiral sector. In the above example, we find that  $c_1^+$  in (71) is identically zero, but there exists a single non-zero solution of  $(c_1^-, c_2^+, c_2^-)$  satisfying (72). To see this, let us notice that only two components of  $\psi_i^\pm$  are independent when  $\psi_i^\pm$  is an eigenstate of  $\Gamma$ . Hence, we obtain two independent linear equations from (72). Solving these linear equations, we have a unique solution  $(c_1^-, c_2^+, c_2^-)$  of (72) up to a overall normalization factor. This result means that no ABS exists in the  $\Gamma = 1$  sector but a single ABS in the  $\Gamma = -1$  sector. Thus,  $N_0^{(+)} = 0$  and  $N_0^{(-)} = 1$ . In a similar manner, we can solve (70) for other  $k_y$ s'. In general, we find that if one of the chiral sectors consists of three (four) wave functions, we have a single non-trivial solution (a pair of non-trivial solutions) of (70). In Table IV, we summarize the number  $N_0^{(\pm)}$  of dispersionless ABS in each sector obtained in this manner. Comparing with the topological number  $W(k_y)$  given in (59) and (60), we find that our result agrees with the index theorem (17) exactly.

In a similar manner, we can also construct the zero energy ABSs on the surface of the two-dimensional semi-infinite  $d_{xy} + p$  wave Rashba superconductor on  $x < 0$ . In comparison with the ABS of the semi-infinite superconductor on  $x > 0$ , the chirality of the ABS is found to be opposite. Thus we find that the index theorem (18) holds in this case.

We notice here that the zero energy bound state for  $k_2 > |k_y| > k_1$  is a Majorana edge mode. The wave function for the zero energy edge state  $\Psi_m(k_y)$  can be written as  ${}^T\Psi_m(k_y) = (u_1(k_y), u_2(k_y), v_1(k_y), v_2(k_y))$  where

$$u_1(k_y) = -i\sigma v_2(k_y) = \frac{(\alpha f_1 - \beta_1 f_2) \exp(ik_y y - i\frac{\pi}{4})}{\sqrt{\sigma\alpha}} \quad (73)$$

$$u_2(k_y) = i\sigma v_1(k_y) = \frac{(f_1 + \beta_2 f_2) \exp(ik_y y - i\frac{\pi}{4})}{\sqrt{\sigma\alpha}} \quad (74)$$

with  $\alpha = (k_y - \sqrt{k_y^2 - k_1^2})/k_1$ ,  $\beta_1 = (\alpha k_y/k_2 + 1)$ ,  $\beta_2 = (\alpha + k_y/k_2)$  and  $\sigma = \text{sgn}(k_y)$ . The functions  $f_1$  and  $f_2$  decays exponentially as a function of  $x$  and are even function of  $k_y$ . The Bogoliubov quasiparticle creation operator for this state is constructed in the usual way as  $\gamma^\dagger(k_y) = u_1(k_y)c_\uparrow^\dagger(k_y) + u_2(k_y)c_\downarrow^\dagger(k_y) + v_1(k_y)c_\uparrow(-k_y) + v_2(k_y)c_\downarrow(-k_y)$ . Since  $u_1(k_y) = v_1^*(-k_y)$  and  $u_2(k_y) = v_2^*(-k_y)$  are satisfied, it is possible to verify that  $\gamma^\dagger(k_y) = \gamma(-k_y)$ . This means the generation of Majorana bound state at the edge for  $k_2 > |k_y| > k_1$ . A similar Majorana bound state also appears for  $\Delta_s > \Delta_t$  and  $k_2 > |k_y| > k_1$ .

Unlike Majorana Fermions studied before, the present single branch of Majorana bound state is realized with time reversal symmetry. The TRI Majorana edge mode has the following three characteristics. a) It has a unique flat dispersion: To be consistent with the time-reversal invariance, the single branch of zero mode should be symmetric under  $k_y \rightarrow -k_y$ . Therefore, by taking into account the particle-hole symmetry as well, the flat dispersion is required. On the other hand, the conventional time-reversal breaking Majorana has a linear dispersion. b) The spin-orbit coupling is necessary to obtain the TRI Majorana edge mode. Without spin-orbit coupling, the TRI Majorana edge mode vanishes. c) The TRI Majorana edge mode is topologically stable under small deformations of the Hamiltonian (49). The topological stability is ensured by the topological invariant  $W(k_y)$ .

## 2. $Z_2$ topological number and anisotropic response to the Zeeman magnetic field

In this section, we would like to point out that the time-reversal invariant Majorana fermion is also characterized by another topological number taking a  $\mathbf{Z}_2$  value. The  $\mathbf{Z}_2$  topological number explains the anisotropic response of the Majorana fermion to the Zeeman magnetic field found in Ref.<sup>107,108</sup>.

For a  $d_{xy} + p$ -wave superconductor, the BdG Hamiltonian has the following symmetry,

$$\mathcal{C}'\mathcal{H}(k_x, k_y)\mathcal{C}'^{-1} = -\mathcal{H}^*(-k_x, k_y), \quad \mathcal{C}' = \begin{pmatrix} 0 & -i\sigma_y \\ i\sigma_y & 0 \end{pmatrix}. \quad (75)$$

Regarding  $k_y$  as a parameter, we can consider this as the particle-hole symmetry in one dimension. Thus the  $\mathbf{Z}_2$  topological number can be introduced in a similar manner as shown in Ref.<sup>67</sup>. As seen from Appendix C, the  $\mathbf{Z}_2$  topological number is given by  $(-1)^{\nu(k_y)}$

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(a)  $\Delta_s > \Delta_t$

$k_y$	$\Gamma = 1$ sector	$\Gamma = -1$ sector	$N_0^{(+)}$	$N_0^{(-)}$	$N_0^{(+)} - N_0^{(-)}$	$W(k_y)$	$(-1)^{\nu(k_y)}$
$k_y > k_2$	$\psi_1^+, \psi_2^+$	$\psi_1^-, \psi_2^-$	0	0	0	0	1
$k_2 > k_y > k_1$	$\psi_1^+$	$\psi_1^-, \psi_2^+, \psi_2^-$	0	1	-1	1	-1
$k_1 > k_y > 0$	-	$\psi_1^+, \psi_1^-, \psi_2^+, \psi_2^-$	0	2	-2	2	1
$0 > k_y > -k_1$	$\psi_1^+, \psi_1^-, \psi_2^+, \psi_2^-$	-	2	0	2	-2	1
$-k_1 > k_y > -k_2$	$\psi_1^-, \psi_2^+, \psi_2^-$	$\psi_1^+$	1	0	1	-1	-1
$-k_2 > k_y$	$\psi_1^-, \psi_2^-$	$\psi_1^+, \psi_2^+$	0	0	0	0	1

(b)  $\Delta_t > \Delta_s$

$k_y$	$\Gamma = 1$ sector	$\Gamma = -1$ sector	$N_0^{(+)}$	$N_0^{(-)}$	$N_0^{(+)} - N_0^{(-)}$	$W(k_y)$	$(-1)^{\nu(k_y)}$
$k_y > k_2$	$\psi_1^+, \psi_2^-$	$\psi_1^-, \psi_2^+$	0	0	0	0	1
$k_2 > k_y > k_1$	$\psi_1^+, \psi_2^+, \psi_2^-$	$\psi_1^-$	1	0	1	-1	-1
$k_1 > k_y > 0$	$\psi_2^+, \psi_2^-$	$\psi_1^+, \psi_1^-$	0	0	0	0	1
$0 > k_y > -k_1$	$\psi_1^+, \psi_1^-$	$\psi_2^+, \psi_2^-$	0	0	0	0	1
$-k_1 > k_y > -k_2$	$\psi_1^-$	$\psi_1^+, \psi_2^+, \psi_2^-$	0	1	-1	1	-1
$-k_2 > k_y$	$\psi_1^-, \psi_2^+$	$\psi_1^+, \psi_2^-$	0	0	0	0	1

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TABLE IV: The zero energy ABSs of the semi-infinite  $d_{xy} + p$ -wave Rashba superconductor on  $x > 0$ . In (a), we consider the spin-singlet dominant Cooper pair,  $\Delta_s > \Delta_t$ , and in (b) the spin-triplet dominant one,  $\Delta_t > \Delta_s$ . In the second and third columns, the chirality of each wave function  $\psi_i^\pm$  in (61) is summarized. As is explained in the text, the numbers  $N_0^{(\pm)}$  of the zero energy ABSs with  $\Gamma = \pm 1$  are determined from the chirality. For comparison, we also show the topological number  $W(k_y)$  given in (59) and (60). In both of the case (a) and (b), the results agree with the index theorem (17) excellently.

with

$$\nu(k_y) = \frac{1}{\pi} \int_0^\infty dk_x A_x(\mathbf{k}). \quad (76)$$

Here  $A_x(\mathbf{k})$  is the “gauge field” defined by the bulk wave function  $|u_n(\mathbf{k})\rangle$ ,

$$A_x(\mathbf{k}) = i \sum_n \langle u_n(\mathbf{k}) | \partial_{k_x} u_n(\mathbf{k}) \rangle. \quad (77)$$

Then the integral can be evaluated as

$$(-1)^{\nu(k_y)} = \text{sgn} \left[ (k_y^2/2m - \mu)^2 - (\lambda k_y)^2 \right]. \quad (78)$$

(See Eq.(C14).) From this, it is found that the  $\mathbf{Z}_2$  topological number is non-trivial, i.e.  $(-1)^{\nu(k_y)} = -1$ , in the region  $k_1 < |k_y| < k_2$  where the dispersionless Majorana fermion exists. Therefore, in addition to  $W(k_y)$ , the  $\mathbf{Z}_2$  topological number  $(-1)^{\nu(k_y)}$  also ensures the topological stability of the dispersionless Majorana fermion.

The merit of the  $\mathbf{Z}_2$  topological invariant is evident if we apply a Zeeman magnetic field. In the presence of Zeeman magnetite field, the chiral symmetry (7) is broken since it is a combination of the particle-hole symmetry and the time-reversal symmetry, and the Zeeman magnetic field breaks the time-reversal invariance. This implies that the topological protection of the gapless state discussed in Sec.III does not work in the presence of a Zeeman magnetic field. In addition, the topological number  $W(k_y)$  cannot be defined without the chiral symmetry.

On the other hand, the symmetry (75) survives even in the presence of the Zeeman magnetic field if we apply it in the  $y$ -direction. Indeed, for the  $d_{xy} + p$ -wave superconductor, we can show that the BdG Hamiltonian

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} \varepsilon(\mathbf{k}) + \mathbf{g}(\mathbf{k}) \cdot \boldsymbol{\sigma} - \mu_B H_y \sigma_y & \hat{\Delta}(\mathbf{k}) \\ \hat{\Delta}^\dagger(\mathbf{k}) & -\varepsilon(\mathbf{k}) + \mathbf{g}(\mathbf{k}) \cdot \boldsymbol{\sigma}^* + \mu_B H_y \sigma_y^* \end{pmatrix} \quad (79)$$

in the presence of the Zeeman magnetic field  $H_y$  in the  $y$ -direction satisfies (75). In a similar manner, we can introduce the  $\mathbf{Z}_2$  invariant, and we obtain

$$(-1)^{\nu(k_y)} = \text{sgn} \left[ (k_y^2/2m - \mu)^2 - (\lambda k_y)^2 - (\mu_B H_y)^2 \right]. \quad (80)$$

(See Eq. (C15).) Thus, the  $\mathbf{Z}_2$  number remains non-trivial in the region where the dispersionless Majorana fermion exists. In fact, the region of  $k_y$  in which the  $\mathbf{Z}_2$  topological number is non-trivial is extended in the presence of  $H_y$ , which suggests that the magnetic field in the  $y$ -direction stabilizes the dispersionless Majorana fermion. This is a peculiar property that is not seen in other dispersionless ABSs. From the bulk-edge correspondence,

we can conclude that the time-reversal invariant dispersionless Majorana fermion survives even in the presence of the Zeeman magnetic field if we apply it in the  $y$ -direction.

Here we notice that the  $\mathbf{Z}_2$  number is very sensitive to the direction of the Zeeman magnetic field we considered. While it is well defined in the presence of a magnetic field in the  $y$ -direction, it becomes meaningless if we apply a magnetic field in the other directions since in the latter case the symmetry (75) is broken. Therefore, the dispersionless Majorana fermion is also very sensitive to the direction of a magnetic field, which is consistent with the surface density of states calculated in Ref.<sup>107,108</sup>.

## VI. INDEX THEOREMS: A PROOF OF BULK-EDGE CORRESPONDENCE

Finally, we would like to prove the index theorems, (17), (18), (28) and (29).

### A. Strategy

Before going into the details, we would like to outline our strategy. In order to prove the index theorems, we introduce an adiabatic parameter  $a$  in the Plank constant  $\hbar$ ,

$$\hbar = a\hbar_0, \tag{81}$$

where  $\hbar_0$  denotes an original value of the Plank constant. When  $a \rightarrow 0$ , we have a classical limit of  $\hbar \rightarrow 0$ , and when  $a = 1$ , the system returns to the original.

We will first consider the semi-classical limit  $\hbar \ll 1$  ( $a \ll 1$ ). Using the WKB approximation, we prove the index theorems in the following sections. ((94) and (96) in Sec.VIB, and (122) and (125) in Sec.VIC, respectively.)

Then we adiabatically increase  $a \rightarrow 1$  until  $\hbar$  goes back to the original value  $\hbar_0$ . From the argument in Sec.III, we notice here that  $N_0^{(+)} - N_0^{(-)}$  cannot change in this process. Indeed, in order to change  $N_0^{(+)} - N_0^{(-)}$ , we need a continuum mode which closes the gap at the corresponding  $\mathbf{k}_{\parallel}$ , but we have a gap in the bulk from the assumption. A new state might appear near the boundary, but it should have a discrete spectrum for a fixed  $\mathbf{k}_{\parallel}$  since it is localized near the boundary. Thus, the boundary state cannot change the value of  $N_0^{(+)} - N_0^{(-)}$  as well. Therefore, the index theorems in the semi-classical limit remain to hold even when  $\hbar$  goes back to the original value.

We would like to emphasize here that our strategy adapted here provides a general framework to prove the bulk-edge correspondence: For any topological state (of non-interacting systems), a mismatch of the topological number on the boundary results in a gap closing point near the boundary, in the classical limit ( $a = 0$ ). Then, by using the WKB quantization of the gap closing point, an gapless edge state is obtained semi-classically ( $a \ll 1$ ). From the existence of a gap in the bulk, the edge state is stable against an adiabatic change of  $a$ , thus we can conclude the existence of the edge state in the original theory ( $a = 1$ ).

## B. $2 \times 2$ BdG Hamiltonian

In this subsection, we prove (28) and (29).

To make a boundary of a superconductor, let us introduce a confining potential  $V(x)$  illustrated in Fig.8,

$$\mathcal{H}_{2 \times 2}(\mathbf{k}) \rightarrow \mathcal{H}_{2 \times 2}(\mathbf{k}, x) = \begin{pmatrix} \varepsilon(\mathbf{k}) + V(x) & \Delta(\mathbf{k}) \\ \Delta(\mathbf{k}) & -\varepsilon(\mathbf{k}) - V(x) \end{pmatrix}. \quad (82)$$

We assume that the confining potential  $V(x)$  is steep enough near the edge. Now we will prove the index theorem (28) for the BdG Hamiltonian (82).

First, we use the WKB approximation to count the zero energy ABSs. For this purpose, it is convenient to solve  $\mathcal{H}_{2 \times 2}(\mathbf{k}, x)^2 v = E^2 v$  instead of the original BdG equation  $\mathcal{H}_{2 \times 2}(\mathbf{k}, x)u = Eu$ . The zero energy states for these two equations are the same as is shown in Appendix.A.

In the presence of the confining potential,  $\mathcal{H}_{2 \times 2}(\mathbf{k}, x)^2$  is given by

$$\mathcal{H}_{2 \times 2}(\mathbf{k}, x)^2 = \begin{pmatrix} (\varepsilon(\mathbf{k}) + V(x))^2 + \Delta(\mathbf{k}) & [V(x), \Delta(\mathbf{k})] \\ -[V(x), \Delta(\mathbf{k})] & (\varepsilon(\mathbf{k}) + V(x))^2 + \Delta(\mathbf{k})^2 \end{pmatrix}. \quad (83)$$

Here  $k_x$  should be treated as  $-i\hbar\partial_x$  in the above. Then noting that

$$[V(x), \Delta(\mathbf{k})] = \frac{\partial V}{\partial x}[x, k_x] \frac{\partial \Delta}{\partial k_x} + O(\hbar^2) = i\hbar \frac{\partial V}{\partial x} \frac{\partial \Delta}{\partial k_x} + O(\hbar^2). \quad (84)$$

we have

$$\mathcal{H}_{2 \times 2}(\mathbf{k}, x)^2 = [(\varepsilon(\mathbf{k}) + V(x))^2 + \Delta(\mathbf{k})^2] \mathbf{1}_{2 \times 2} - \hbar \frac{\partial V}{\partial x} \frac{\partial \Delta}{\partial k_x} \sigma_y + O(\hbar^2). \quad (85)$$

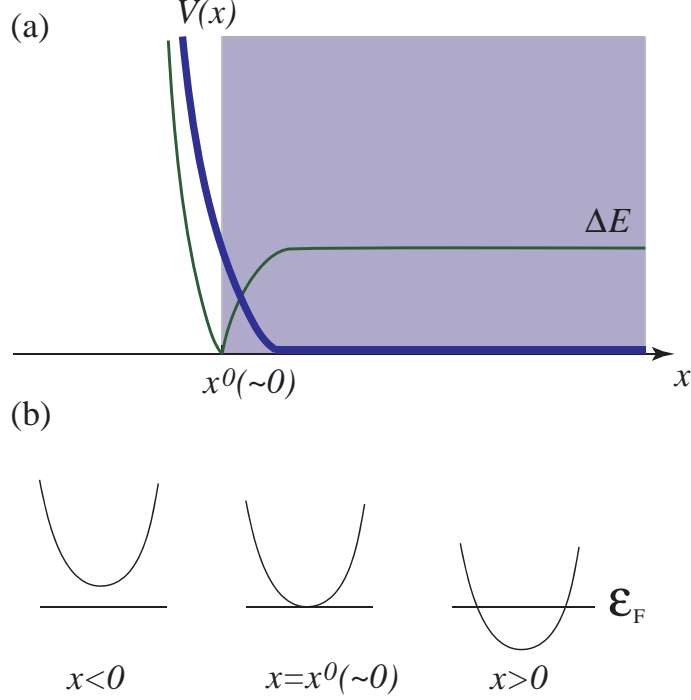


FIG. 8: (color online) (a) A semi-infinite superconductor on  $x > 0$ . The thick curve denotes the confining potential  $V(x)$ , and the thin curve a gap of the system in the classical limit. If Eq. (87) is satisfied, the gap  $\Delta E$  in the classical limit closes near the edge at  $x = 0$ . (b) The corresponding normal dispersion of electrons. Inside the superconductor ( $x > 0$ ), the system supports the Fermi surface, but outside the superconductor ( $x < 0$ ), the system becomes a band insulator. Correspondingly,  $\Delta E$  is a superconducting gap for  $x > 0$ , and  $\Delta E$  is a band gap ( $\sim V(x)$ ) for  $x < 0$ .

In the classical limit ( $\hbar \rightarrow 0$ ) of the WKB approximation, the energy spectrum is given by the first term of the right hand side of (85),

$$E^2 = (\varepsilon(\mathbf{k}) + V(x))^2 + \Delta(\mathbf{k})^2, \quad (86)$$

where  $\mathbf{k}$  and  $x$  should be considered as  $c$ -numbers. For a fixed  $\mathbf{k}_{\parallel}$ , we have a zero energy state if  $(k_x, x) = (k_x^0, x^0)$  satisfies

$$\varepsilon(k_x^0, \mathbf{k}_{\parallel}) + V(x^0) = 0, \quad \Delta(k_x^0, \mathbf{k}_{\parallel}) = 0. \quad (87)$$

Let us now take into account the leading order correction of  $\hbar$ . Near the zero  $(k_x^0, x^0)$

satisfying (87), we obtain

$$\begin{aligned}\varepsilon(\mathbf{k}) + V(x) &= \left( \frac{\partial V(x)}{\partial x} \right)_{x=x^0} (x - x^0) + \dots, \\ \Delta(\mathbf{k}) &= \left( \frac{\partial \Delta(\mathbf{k})}{\partial k_x} \right)_{k_x=k_x^0} (k_x - k_x^0) + \dots,\end{aligned}\quad (88)$$

thus the first term of (85) is evaluated as a harmonic oscillator,

$$[(\varepsilon(\mathbf{k}) + V(x))^2 + \Delta(\mathbf{k})^2] = \left( \frac{\partial V}{\partial x} \right)_{x=x^0}^2 (x - x^0)^2 + \left( \frac{\partial \Delta}{\partial k_x} \right)_{k_x=k_x^0}^2 (k_x - k_x^0)^2 + \dots \quad (89)$$

From the Bohr-Sommerfeld quantization condition, it leads to

$$[(\varepsilon(\mathbf{k}) + V(x))^2 + \Delta(\mathbf{k})^2] = 2\hbar \left| \frac{\partial V}{\partial x} \right|_{x=x^0} \left| \frac{\partial \Delta}{\partial k_x} \right|_{k_x=k_x^0} \left( n + \frac{1}{2} \right) + O(\hbar^2), \quad (90)$$

with  $n = 0, 1, 2, \dots$ . The second term in (85) is evaluated as the expectation value for the WKB wave function,

$$-\hbar \left\langle \frac{\partial V}{\partial x} \frac{\partial \Delta}{\partial k_x} \right\rangle_0 \sigma_y = -\hbar \left( \frac{\partial V}{\partial x} \right)_{x=x^0} \left( \frac{\partial \Delta}{\partial k_x} \right)_{k_x=k_x^0} \sigma_y, \quad (91)$$

where we have used the fact that the WKB wave function has a sharp peak at  $x = x^0$  and  $k_x = k_x^0$ . Combining (90) and (91), we obtain

$$\mathcal{H}_{2 \times 2}(\mathbf{k}, x)^2 = 2\hbar \left| \frac{\partial V}{\partial x} \right|_{x=x^0} \left| \frac{\partial \Delta}{\partial k_x} \right|_{k_x=k_x^0} \left( n + \frac{1}{2} \right) \mathbf{1}_{2 \times 2} - \hbar \left( \frac{\partial V}{\partial x} \right)_{x=x^0} \left( \frac{\partial \Delta}{\partial k_x} \right)_{k_x=k_x^0} \sigma_y. \quad (92)$$

For a semi-infinite superconductor on  $x > 0$ , the confining potential satisfies  $(\partial V / \partial x)_{x=x^0} < 0$ . Therefore Eq.(92) yields a zero energy solution with chirality  $\gamma$  ( $\equiv$  an eigenvalue of  $\sigma_y$ ) given by

$$\gamma = -\text{sgn} \left( \frac{\partial \Delta}{\partial k_x} \right)_{k_x=k_x^0}. \quad (93)$$

Counting the zero energy states from all  $(k_x^0, x^0)$ s satisfying (87), we obtain

$$n_0^{(+)} - n_0^{(-)} = - \sum \text{sgn} \left( \frac{\partial \Delta}{\partial k_x} \right)_{k_x=k_x^0}, \quad (94)$$

where the summation is taken for  $(k_x^0, x^0)$  satisfying (87).

Here we can show that (94) is nothing but the index theorem (28): First, we note that if and only if  $\varepsilon(\mathbf{k}) < 0$ , there exists a  $x$  satisfying  $\varepsilon(\mathbf{k}) + V(x) = 0$ . Thus we can rewrite (94) as

$$n_0^{(+)} - n_0^{(-)} = - \sum_{\Delta(k_x^0, \mathbf{k}_{\parallel})=0, \varepsilon(k_x^0, \mathbf{k}_{\parallel}) < 0} \text{sgn} \left( \frac{\partial \Delta}{\partial k_x} \right)_{k_x=k_x^0}, \quad (95)$$



As is shown in Sec.B 1, the right hand side of the above equation is equal to  $-w(\mathbf{k}_{\parallel})$ , thus we have the index theorem

$$n_0^{(-)} - n_0^{(+)} = w(\mathbf{k}_{\parallel}). \quad (96)$$

in the leading order in the WKB approximation.

While we have derived Eq. (96) in the leading order of the WKB approximation, we can find that no further correction exists: As was discussed in Sec.III, any small perturbation preserving the chiral symmetry cannot change  $n_0^{(+)} - n_0^{(-)}$  unless the bulk energy gap closes. Therefore, a higher order correction might change each of  $n_0^{(+)}$  or  $n_0^{(-)}$ , but it cannot change their difference  $n_0^{(+)} - n_0^{(-)}$ . This means that Eq.(96) is exact. (See also the discussions in Sec.VI A.)

In a similar manner, we can prove the index theorem (29) for a semi-infinite superconductor on  $x < 0$ . Following the same argument above, we obtain (92) again. However, in comparison with the semi-infinite superconductor on  $x > 0$ , the sign of  $(\partial V/\partial x)_{x=x^0}$  is reversed for a semi-infinite superconductor on  $x < 0$ , so the chirality  $\gamma$  of the zero energy state is also reversed

$$\gamma = \text{sgn} \left( \frac{\partial \Delta}{\partial k_x} \right)_{k_x=k_x^0}. \quad (97)$$

Thus we obtain

$$n_0^{(+)} - n_0^{(-)} = \sum \text{sgn} \left( \frac{\partial \Delta}{\partial k_x} \right)_{k_x=k_x^0}, \quad (98)$$

where the summation is taken for  $(k_x^0, x^0)$  satisfying (87). This leads to

$$n_0^{(+)} - n_0^{(-)} = w(\mathbf{k}_{\parallel}), \quad (99)$$

which is exact again for the same reason above.

### C. General case

Now, we prove the index theorems (17) and (18) for general time-reversal invariant BdG Hamiltonian.

First let us consider the index theorem (17) for a semi-infinite superconductor on  $x > 0$ . To realize the semi-infinite superconductor, we introduce a confining potential  $V(x)$  in a

similar manner as Sec.VIB (See also Fig.8),

$$\mathcal{H}(\mathbf{k}) \rightarrow \mathcal{H}(\mathbf{k}, x) = \begin{pmatrix} \hat{\mathcal{E}}(\mathbf{k})_{\alpha\alpha'} + V(x)\delta_{\alpha\alpha'} & \hat{\Delta}(\mathbf{k})_{\alpha\alpha'} \\ \hat{\Delta}^\dagger(\mathbf{k})_{\alpha\alpha'} & -\hat{\mathcal{E}}^T(-\mathbf{k})_{\alpha\alpha'} - V(x)\delta_{\alpha\alpha'} \end{pmatrix}, \quad (100)$$

where  $V(x) = 0$  inside the superconductor ( $x > 0$ ). We suppose a sharp edge where the confining potential  $V(x)$  is very steep near the edge ( $x = 0$ ).

In the classical limit  $\hbar \rightarrow 0$ ,  $k_x$  and  $x$  commute with each other, thus we can treat them as  $c$ -numbers. Then, considering  $x$  as a parameter, we define the winding number  $W(\mathbf{k}_\parallel, x)$  in a manner similar to Eq.(11),

$$\begin{aligned} W(\mathbf{k}_\parallel, x) &= -\frac{1}{4\pi i} \int d\mathbf{k}_\perp \text{tr} [\Gamma \mathcal{H}^{-1}(\mathbf{k}, x) \partial_{\mathbf{k}_\perp} \mathcal{H}(\mathbf{k}, x)] \\ &= \frac{1}{2\pi} \text{Im} \left[ \int d\mathbf{k}_\perp \partial_{\mathbf{k}_\perp} \ln \det \hat{q}(\mathbf{k}, x) \right], \end{aligned} \quad (101)$$

where  $\hat{q}(\mathbf{k}, x) = i[\hat{\mathcal{E}}(\mathbf{k}) + V(x)]U^\dagger - \hat{\Delta}(\mathbf{k})$  with  $U$  in Eq.(4), and  $\mathbf{k}_\perp = k_x$ . The line integral in the above is defined in the same way as Eq.(11).

Here we find that  $W(\mathbf{k}_\parallel, x)$  is identical to  $W(\mathbf{k}_\parallel)$  inside the superconductor  $x > 0$ ,

$$W(\mathbf{k}_\parallel, x) = W(\mathbf{k}_\parallel), \quad \text{for } x > 0, (x \not\sim 0), \quad (102)$$

since  $V(x) = 0$  there. We also find that  $W(\mathbf{k}_\perp, x)$  becomes zero outside the superconductor,

$$W(\mathbf{k}_\parallel, x) = 0 \quad \text{for } x < 0, (x \not\sim 0), \quad (103)$$

since we have a vacuum there. Therefore, if the bulk superconductor supports a non-zero winding number  $W(\mathbf{k}_\parallel) \neq 0$ , then the value of  $W(\mathbf{k}_\parallel, x)$  must be changed near the edge ( $x = 0$ ). This immediately implies that when  $W(\mathbf{k}_\parallel) \neq 0$ , a gap of the system closes near the edge in the classical limit: Since  $W(\mathbf{k}_\parallel, x)$  is a topological number, it changes only when the line integral is ill-defined. Then this occurs only when  $\det \hat{q}(\mathbf{k}, x) = 0$ , which means a gap closing of the system in the classical limit.

To examine how  $W(\mathbf{k}_\parallel, x)$  changes, we diagonalize  $\hat{q}(\mathbf{k}, x)$  as

$$\begin{aligned} \hat{q}(\mathbf{k}, x) &= A(\mathbf{k}, x) \Lambda(\mathbf{k}, x) B^\dagger(\mathbf{k}, x), \\ \hat{q}^\dagger(\mathbf{k}, x) &= B(\mathbf{k}, x) \Lambda^*(\mathbf{k}, x) A^\dagger(\mathbf{k}, x), \end{aligned} \quad (104)$$

where  $\Lambda(\mathbf{k}, x) = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_N)$  with  $\lambda_i$  the eigenvalue of  $\hat{q}(\mathbf{k}, x)$ , and  $A(\mathbf{k}, x)$  and  $B(\mathbf{k}, x)$  are  $N \times N$  matrices satisfying

$$A(\mathbf{k}, x) B^\dagger(\mathbf{k}, x) = \mathbf{1}_{N \times N}. \quad (105)$$

(Here we assume that  $\hat{q}(\mathbf{k}, x)$  is an  $N \times N$  matrix. See Appendix E for details.) Since Eq.(104) yields that  $\det \hat{q}(\mathbf{k}, x) = \det \Lambda(\mathbf{k}, x) = \prod_n \lambda_n(\mathbf{k}, x)$ , the winding number  $W(\mathbf{k}, x)$  is recast into

$$W(\mathbf{k}_{\parallel}, x) = \frac{1}{2\pi} \text{Im} \left[ \sum_{n=1}^N \int d\mathbf{k}_{\perp} \partial_{\mathbf{k}_{\perp}} \ln \lambda_n(\mathbf{k}, x) \right]. \quad (106)$$

Thus the line integral of  $W(\mathbf{k}_{\parallel}, x)$  is ill-defined, when some of the eigenvalues  $\lambda_n(\mathbf{k}, x)$  have a zero.

Now suppose that  $\lambda_n(\mathbf{k}, x)$  has a zero at  $(x, k_x) = (x^0, k_x^0)$ ,

$$\begin{aligned} \lambda_n &= \alpha e^{i\beta} (x - x^0) + \gamma e^{i\delta} (k_x - k_x^0) + \cdots, \\ &= \alpha e^{i\beta} [(x - x^0) + (\gamma/\alpha) e^{i(\delta-\beta)} (k_x - k_x^0)] + \cdots, \end{aligned} \quad (107)$$

where  $\alpha, \beta, \gamma$  and  $\delta$  are real constants. We notice here that  $\alpha$  is very large since it is proportional to  $(\partial V/\partial x)_{x=x^0}$  and  $V(x)$  is steep near the edge. Thus we can neglect the real part of  $(\gamma/\alpha) e^{i(\delta-\beta)} (k_x - k_x^0)$ , and obtain

$$\lambda_n = \alpha e^{i\beta} [(x - x^0) + i\eta (k_x - k_x^0)] + \cdots, \quad (108)$$

with  $\eta = (\gamma/\alpha) \sin(\delta - \beta)$ . This zero changes the value of the winding number  $W(\mathbf{k}_{\parallel}, x)$  as follows. Consider the line integrals near the zero along  $x = x^i$  illustrated in Fig 9,

$$\int_{x=x^i} dk_x \partial_{k_x} \ln \lambda_n(\mathbf{k}, x) \quad (i = 1, 2) \quad (109)$$

with  $x^1 < x^0 < x^2$ . The difference of these line integrals is evaluated as

$$\begin{aligned} & \int_{x=x^2} dk_x \partial_{k_x} \ln \lambda_n(\mathbf{k}, x) - \int_{x=x^1} dk_x \partial_{k_x} \ln \lambda_n(\mathbf{k}, x) \\ &= \oint_C dk_x \partial_{k_x} \ln \lambda_n(\mathbf{k}, x) \\ &= 2\pi i \text{sgn}[\eta], \end{aligned} \quad (110)$$

thus from Eq.(106), we have

$$W(\mathbf{k}_{\parallel}, x^2) - W(\mathbf{k}_{\parallel}, x^1) = \text{sgn}[\eta]. \quad (111)$$

In a similar manner, we can consider other zeros of the eigenvalues of  $\hat{q}(\mathbf{k}, x)$ . Then summing up all contribution of these zeros  $(x^{0(i)}, k_x^{0(i)})$  of  $\lambda_{n(i)}$  ( $i = 1, \dots, M$ ), we have

$$W(\mathbf{k}_{\parallel}) = \sum_{i=1}^M \text{sgn}[\eta_i], \quad (112)$$

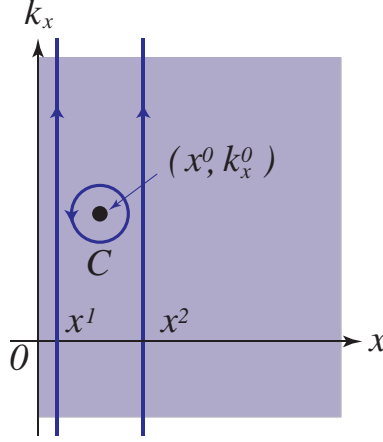


FIG. 9: (color online) A zero  $(x^0, k_x^0)$  of  $\lambda_n$  near the edge of a semi-infinite superconductor on  $x > 0$ .

where  $\eta_i$  is given by

$$\lambda_{n(i)} = \alpha_i e^{i\beta_i} [(x - x^{0(i)}) + i\eta_i(k_x - k_x^{0(i)})] + \dots, \quad (113)$$

with real functions  $\alpha_i$  and  $\beta_i$ . Since  $\det \mathcal{H}(\mathbf{k}, x)$  around the zero  $(x^{0(i)}, k_x^{0(i)})$  is evaluated as

$$\begin{aligned} \det \mathcal{H}(\mathbf{k}, x) &\propto \det \hat{q}(\mathbf{k}, x) \hat{q}^\dagger(\mathbf{k}, x) \\ &= \prod_n |\lambda_n(\mathbf{k}, x)|^2 \\ &\sim [(x - x^{0(i)})^2 + \eta_i^2(k_x - k_x^{0(i)})^2], \end{aligned} \quad (114)$$

the classical spectrum around each zero is a harmonic oscillator.

Let us now take into account the quantum corrections. In the leading order correction of  $\hbar$ , the classical spectrum of a harmonic oscillator around each zero is quantized. To see whether the zero energy state survives or not after the quantization, let us examine the BdG equation for the zero energy state,

$$\mathcal{H}(\mathbf{k}, x)u_0 = 0, \quad (115)$$

which is equivalent to

$$\hat{q}(\mathbf{k}, x)\phi_0 = 0, \quad \hat{q}^\dagger(\mathbf{k}, x)\psi_0 = 0, \quad (116)$$

with

$$u_0 = U_\Gamma \begin{pmatrix} \psi_0 \\ \phi_0 \end{pmatrix}. \quad (117)$$

Substituting the following expression

$$\phi_0 = a_{n(i)}(k_x^{0(i)}, \mathbf{k}_{\parallel}, x^{0(i)})f(x), \quad \psi_0 = b_{n(i)}(k_x^{0(i)}, \mathbf{k}_{\parallel}, x^{0(i)})g(x), \quad (118)$$

into Eq.(116), we find that

$$\begin{aligned} [x - x^{0(i)} + i\eta_i(k_x - k_x^{0(i)})] f(x) &= 0, \\ [x - x^{0(i)} - i\eta_i(k_x - k_x^{0(i)})] g(x) &= 0, \end{aligned} \quad (119)$$

around the zero  $(x^{0(i)}, k_x^{0(i)})$ . Here  $a_n(\mathbf{k}, x)$  and  $b_n(\mathbf{k}, x)$  are the eigenfunctions of  $q(\mathbf{k}, x)$  and  $q^\dagger(\mathbf{k}, x)$  in the classical limit, defined in Appendix E. Replacing  $k_x$  with  $-i\hbar\partial_x$ , we can easily solve Eq.(119), which reads

$$\begin{aligned} f(x) &= f_0 \exp \left[ i \frac{k_x^{0(i)}}{\hbar} x \right] \exp \left[ \frac{-(x - x^{0(i)})^2}{2\eta_i \hbar} \right], \\ g(x) &= g_0 \exp \left[ i \frac{k_x^{0(i)}}{\hbar} x \right] \exp \left[ \frac{(x - x^{0(i)})^2}{2\eta_i \hbar} \right], \end{aligned} \quad (120)$$

where  $f_0$  and  $g_0$  are constants. Since the normalization condition requires that  $f_0$  is zero if  $\eta_i < 0$ , and  $g_0$  is zero if  $\eta_i > 0$ , the zero energy state has  $\Gamma = 1$  for  $\eta_i < 0$  and  $\Gamma = -1$  for  $\eta_i > 0$ , respectively. (We have used Eq.(8) when applying  $\Gamma$  to  $u_0$  in Eq.(117).) In other words, in the leading order of the WKB quantization, there exists a zero energy state for each zero  $(x^{0(i)}, k_x^{0(i)})$ , and its chirality  $\Gamma$  is given by

$$\Gamma = -\text{sgn}[\eta_i]. \quad (121)$$

From (112), this leads to

$$W(\mathbf{k}_{\parallel}) = N_0^{(-)} - N_0^{(+)}. \quad (122)$$

From the same argument as in Sec.VI B, we can conclude that no higher order correction of  $\hbar$  exists in Eq.(122) again. Then using the argument in Sec.VI A, we conclude that Eq.(122) is an exact result.

In a similar manner, we can derive (18) for a semi-infinite superconductor on  $x < 0$ . As illustrated in Fig.10, for a zero  $(x^0, k_x^0)$  of  $\lambda_n$  near the edge  $x = 0$ , we have again Eq.(110),

$$\int_{x=x^2}^{\infty} dk_x \partial_{k_x} \ln \lambda_n - \int_{x=x^1}^{\infty} dk_x \partial_{k_x} \ln \lambda_n = 2\pi i \text{sgn}[\eta], \quad (123)$$

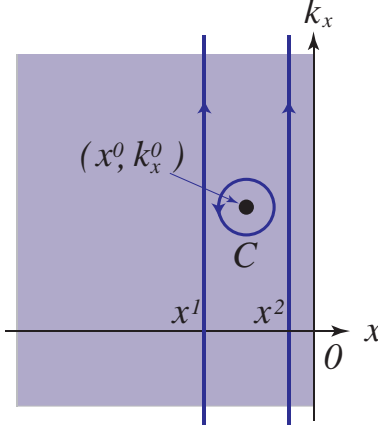


FIG. 10: (color online) A zero  $(x^0, k_x^0)$  of  $\lambda_n$  near the edge of a semi-infinite superconductor on  $x < 0$ .

with  $x^1 < x^0 < x^2$ , but in contrast to the previous case, the line integral along  $x = x^2$  is located at an outer region of the superconductor. Thus the sign of the right hand side of Eq.(112) is reversed,

$$W(\mathbf{k}_{\parallel}) = - \sum_i \text{sgn}[\eta_i], \quad (124)$$

and the following index theorem is obtained

$$W(\mathbf{k}_{\parallel}) = N_0^{(+)} - N_0^{(-)}. \quad (125)$$

From the argument in Sec.VI A, this result holds again beyond the WKB approximation.

## VII. CONCLUSION

In this paper, we have discussed the topology of the ABS with flat dispersion at zero energy which appears on a boundary of time-reversal invariant superconductors. Using the symmetry of the BdG Hamiltonian, we have introduced the topological numbers  $W(\mathbf{k}_{\parallel})$  and  $w(\mathbf{k}_{\parallel})$ , and from the bulk-edge correspondence, topological criteria for the dispersionless ABS were obtained, which are summarized as the index theorems (17), (18), (28) and (29). We have shown that the index theorems correctly predict the existence of the dispersionless ABSs. It has been also clarified that sign change of the gap function is directly related to our topological criterion for superconductors preserving  $S_z$  with simple Fermi surfaces. As

concrete examples, we have also discussed (i)  $d_{xy}$ -wave superconductor, (ii)  $p_x$ -wave superconductor, and (iii)  $d_{xy} + p$ -wave superconductor. All the examples confirms our topological criteria excellently. In the last part of this paper, we provide a general framework to certify the bulk-edge correspondence, and we prove the index theorems.

While we have considered only superconductors in this paper, the index theorems we found can apply to other systems. For example, graphene in the nearest neighbor tight-binding model has chiral symmetry (or sublattice symmetry) similar to (23)<sup>130</sup>, thus the index theorems (28) and (29) hold. In general, our index theorems apply to any non-interacting Hamiltonian with chiral symmetry.

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### Appendix A: basic properties of system with chiral symmetry

Here we summarize the properties of the system with chiral symmetry. Suppose that the Hamiltonian  $\mathcal{H}$  has the chiral symmetry  $\Gamma$

$$\{\mathcal{H}, \Gamma\} = 0, \quad \Gamma^2 = 1. \quad (\text{A1})$$

Then consider the BdG equation

$$\mathcal{H}|u_E\rangle = E|u_E\rangle \quad (\text{A2})$$

First, we would like to show that there exists a one to one correspondence between the solution of (A2) and that of the following equation,

$$\mathcal{H}^2|v_{E^2}\rangle = E^2|v_{E^2}\rangle. \quad (\text{A3})$$

Since it is evident that the solution  $|u_E\rangle$  of (A2) satisfies (A3), here we show only the reverse. Namely, we can construct the solution  $|u_E\rangle$  of (A2) from the solution  $|v_{E^2}\rangle$  of (A3): For  $E^2 \neq 0$ , if  $(\mathcal{H} + E)|v_{E^2}\rangle \neq 0$ , the solution  $|u_E\rangle$  of (A2) is obtained by

$$|u_E\rangle = c(\mathcal{H} + E)|v_{E^2}\rangle \quad (\text{A4})$$

with a normalization constant  $c$ . Then if  $(\mathcal{H} + E)|v_{E^2}\rangle = 0$ , the solution is given by

$$|u_E\rangle = \Gamma|v_{E^2}\rangle. \quad (\text{A5})$$

It is easily found that  $|u_E\rangle$  in (A4) and (A5) has a nonzero norm and satisfies (A2). For  $E^2 = 0$ , we have

$$\mathcal{H}^2|v_0\rangle = 0. \quad (\text{A6})$$

Since this equation implies that

$$\langle v_0|\mathcal{H}^2|v_0\rangle = ||\mathcal{H}|v_0\rangle||^2 = 0, \quad (\text{A7})$$

we obtain

$$\mathcal{H}|v_0\rangle = 0. \quad (\text{A8})$$

Therefore, the zero energy solution  $|u_0\rangle$  is obtained by  $|u_0\rangle = |v_0\rangle$ . Since there exists a one to one correspondence between the solution of (A2) and that of (A3), we examine (A3) instead of (A2) in the following.

Because  $\mathcal{H}^2$  and  $\Gamma$  commute with each other, we can take the solution of (A3) as the eigen state of  $\Gamma$ , simultaneously. Then, it is found that for  $E^2 \neq 0$ , the solution  $|v_{E^2}^+\rangle$  satisfying  $\Gamma|v_{E^2}^+\rangle = |v_{E^2}^+\rangle$  is constructed from the solution  $|v_{E^2}^-\rangle$  satisfying  $\Gamma|v_{E^2}^-\rangle = -|v_{E^2}^-\rangle$  by multiplying  $\mathcal{H}$  from the left,

$$|v_{E^2}^+\rangle = c'\mathcal{H}|v_{E^2}^-\rangle, \quad (\text{A9})$$

where  $c'$  is a normalization constant. In a similar manner, we can construct  $|v_{E^2}^-\rangle$  from  $|v_{E^2}^+\rangle$ . Therefore, for  $E^2 \neq 0$ , the solution of (A3) with the chirality  $\Gamma = 1$  is always paired with the solution with  $\Gamma = -1$ .

On the other hand, for  $E^2 = 0$ , the solution does not form a pair in general. Indeed, as was shown in the above, the solution  $|v_0^-\rangle$  with  $E^2 = 0$  satisfies  $\mathcal{H}|v_0^-\rangle = 0$ , thus Eq.(A9) leads to  $|v_0^+\rangle = 0$ . Thus we do not obtain the paired state in this case.



## Appendix B: Derivation of useful formulas

### 1. Formulas for $w(k_y)$

We first evaluate the integral (26)

$$w(k_y) = \frac{1}{2\pi} \text{Im} \left[ \int dk_x \partial_{k_x} \ln q(\mathbf{k}) \right], \quad (\text{B1})$$

with  $q(\mathbf{k}) = -i\varepsilon(\mathbf{k}) - \Delta(\mathbf{k})$ . To calculate this integral, it is convenient to rewrite this as

$$w(k_y) = -\frac{1}{2\pi} \int dk_x \epsilon^{ab} m_a(\mathbf{k}) \partial_{k_x} m_b(\mathbf{k}), \quad (\text{B2})$$

where

$$m_1(\mathbf{k}) = \frac{\varepsilon(\mathbf{k})}{\sqrt{\varepsilon^2(\mathbf{k}) + \Delta^2(\mathbf{k})}}, \quad m_2(\mathbf{k}) = \frac{\Delta(\mathbf{k})}{\sqrt{\varepsilon^2(\mathbf{k}) + \Delta^2(\mathbf{k})}}. \quad (\text{B3})$$

Then we apply a technique used in Ref.<sup>123,126</sup>. Since the integral (B2) is a topological number, it can not change its value even if we rescale  $\Delta(\mathbf{k})$  as  $a\Delta(\mathbf{k})$  ( $a \leq 1$ ),

$$m_1(\mathbf{k}) \rightarrow \frac{\varepsilon(\mathbf{k})}{\sqrt{\varepsilon^2(\mathbf{k}) + a^2 \Delta^2(\mathbf{k})}}, \quad m_2(\mathbf{k}) \rightarrow \frac{a\Delta(\mathbf{k})}{\sqrt{\varepsilon^2(\mathbf{k}) + a^2 \Delta^2(\mathbf{k})}} \quad (\text{B4})$$

Then when  $a \ll 1$ , except the neighborhoods of the zero of  $\varepsilon(\mathbf{k})$ ,  $m_a(\mathbf{k})$  becomes a constant

$$m_1(\mathbf{k}) \sim \pm 1, \quad m_2(\mathbf{k}) \sim 0. \quad (\text{B5})$$

Thus only the neighborhood of the zero of  $\varepsilon(\mathbf{k})$  contributes the integral. Expanding  $\varepsilon(\mathbf{k})$  and  $\Delta(\mathbf{k})$  around the  $k_x^0$  satisfying  $\varepsilon(k_x^0, k_y) = 0$ ,

$$\varepsilon(\mathbf{k}) = \partial_{k_x} \varepsilon(k_x^0, k_y) (k_x - k_x^0) + \cdots, \quad \Delta(\mathbf{k}) = \Delta(k_x^0, k_y) + \cdots, \quad (\text{B6})$$

we estimate the contribution near the  $k_x^0$  as

$$\frac{1}{2} \text{sgn}[\partial_{k_x} \varepsilon(k_x^0, k_y)] \text{sgn} \Delta(k_x^0, k_y). \quad (\text{B7})$$

Summing up the contribution from  $k_x^0$ 's, we obtain Eq.(27)

$$w(k_y) = \frac{1}{2} \sum_{\varepsilon(k_x^0, k_y)=0} \text{sgn}[\partial_{k_x} \varepsilon(k_x^0, k_y)] \text{sgn} \Delta(k_x^0, k_y). \quad (\text{B8})$$

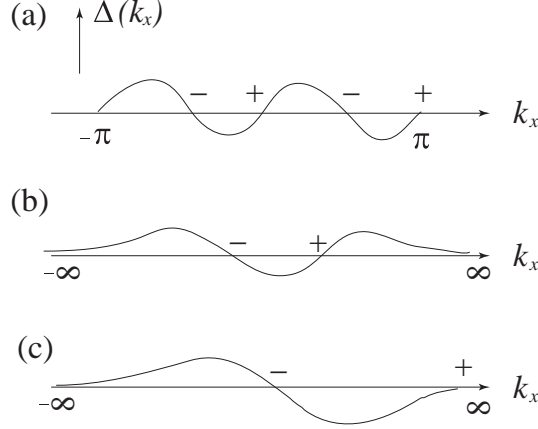


FIG. 11: Examples of  $\Delta(\mathbf{k})$  as a function of  $k_x$ . The symbols  $\pm$  represent the sign of  $\partial_{k_x} \Delta(k_x)$  at  $k_x = k_x^0$  with  $\Delta(k_x^0) = 0$ . (a)  $\Delta(\mathbf{k})$  in a lattice model. From the periodicity in  $k_x$ , Eq.(B10) holds. (b) and (c)  $\Delta(\mathbf{k})$  in a continuum model. Here we regulate  $\Delta(\mathbf{k})$  as  $\Delta(\mathbf{k}) \rightarrow 0$  at  $k_x = \pm\infty$ . In the case (c), we need to take into account the contribution at  $k_x = \infty$  to obtain Eq.(B10).

In a similar manner, we also obtain the following formula by exchanging  $\varepsilon(\mathbf{k})$  with  $\Delta(\mathbf{k})$  in the above,

$$w(k_y) = -\frac{1}{2} \sum_{\Delta(k_x^0, k_y)=0} \text{sgn} [\partial_{k_y} \Delta(k_x^0, k_y)] \text{sgn} \varepsilon(k_x^0, k_y). \quad (\text{B9})$$

As illustrated in Fig.11, the following identity holds in general,

$$\sum_{\Delta(k_x^0, k_y)=0} \text{sgn} [\partial_{k_x} \Delta(k_x^0, k_y)] = 0. \quad (\text{B10})$$

For a lattice model, this equation comes from the periodicity in  $k_x$ , and for a continuum model, this holds from the regularization in which  $\Delta(\mathbf{k})$  at  $k_x = \infty$  is identified with that at  $k_x = -\infty$ . Since the left hand side of Eq.(B10) is rewritten as

$$\begin{aligned} & \sum_{\Delta(k_x^0, k_y)=0} \text{sgn} [\partial_{k_x} \Delta(k_x^0, k_y)] \\ &= \sum_{\Delta(k_x^0, k_y)=0, \varepsilon(k_x^0, k_y)>0} \text{sgn} [\partial_{k_x} \Delta(k_x^0, k_y)] \\ &+ \sum_{\Delta(k_x^0, k_y)=0, \varepsilon(k_x^0, k_y)<0} \text{sgn} [\partial_{k_x} \Delta(k_x^0, k_y)], \end{aligned} \quad (\text{B11})$$

Eq.(B10) leads to

$$\sum_{\Delta(k_x^0, k_y)=0, \varepsilon(k_x^0, k_y)>0} \text{sgn} [\partial_{k_x} \Delta(k_x^0, k_y)] = - \sum_{\Delta(k_x^0, k_y)=0, \varepsilon(k_x^0, k_y)<0} \text{sgn} [\partial_{k_x} \Delta(k_x^0, k_y)] \quad (\text{B12})$$

From this equation, Eq.(B9) is recast into

$$\begin{aligned}
w(k_y) &= -\frac{1}{2} \sum_{\Delta(k_x^0, k_y)=0, \varepsilon(k_x^0, k_y)>0} \text{sgn} [\partial_{k_x} \Delta(k_x^0, k_y)] \\
&+ \frac{1}{2} \sum_{\Delta(k_x^0, k_y)=0, \varepsilon(k_x^0, k_y)<0} \text{sgn} [\partial_{k_x} \Delta(k_x^0, k_y)] \\
&= \sum_{\Delta(k_x^0, k_y)=0, \text{sgn} \varepsilon(k_x^0, k_y)<0} \text{sgn} [\partial_{k_x} \Delta(k_x^0, k_y)].
\end{aligned} \tag{B13}$$

We will use this formula in Sec.VI B.

## 2. Formulas for $W(k_y)$

Here we evaluate the integral (51)

$$W(k_y) = \frac{1}{2\pi} \text{Im} \left[ \int dk_x \partial_{k_x} \ln \det \hat{q}(\mathbf{k}) \right], \tag{B14}$$

with

$$\hat{q}(\mathbf{k}) = [\varepsilon(\mathbf{k}) - i\psi(\mathbf{k})]\sigma_y + [\mathbf{g}(\mathbf{k}) - i\mathbf{d}(\mathbf{k})] \cdot \boldsymbol{\sigma} \sigma_y. \tag{B15}$$

Since the determinant of  $\hat{q}(\mathbf{k})$  is given by

$$\det \hat{q}(\mathbf{k}) = -\varepsilon^2(\mathbf{k}) + \mathbf{g}^2(\mathbf{k}) + \psi^2(\mathbf{k}) - \mathbf{d}^2(\mathbf{k}) - 2i[\mathbf{g}(\mathbf{k}) \cdot \mathbf{d}(\mathbf{k}) - \varepsilon(\mathbf{k})\psi(\mathbf{k})], \tag{B16}$$

the above integral is recast into the same form as (B2) with

$$\begin{aligned}
m_1(\mathbf{k}) &= \frac{2(\mathbf{g}(\mathbf{k}) \cdot \mathbf{d}(\mathbf{k}) - \varepsilon(\mathbf{k})\psi(\mathbf{k}))}{\sqrt{[\varepsilon^2(\mathbf{k}) - \mathbf{g}^2(\mathbf{k}) - \psi^2(\mathbf{k}) + \mathbf{d}^2(\mathbf{k})]^2 + 4[\mathbf{g}(\mathbf{k}) \cdot \mathbf{d}(\mathbf{k}) - \varepsilon(\mathbf{k})\psi(\mathbf{k})]^2}}, \\
m_2(\mathbf{k}) &= \frac{\varepsilon^2(\mathbf{k}) - \mathbf{g}^2(\mathbf{k}) - \psi^2(\mathbf{k}) + \mathbf{d}^2(\mathbf{k})}{\sqrt{[\varepsilon^2(\mathbf{k}) - \mathbf{g}^2(\mathbf{k}) - \psi^2(\mathbf{k}) + \mathbf{d}^2(\mathbf{k})]^2 + 4[\mathbf{g}(\mathbf{k}) \cdot \mathbf{d}(\mathbf{k}) - \varepsilon(\mathbf{k})\psi(\mathbf{k})]^2}}.
\end{aligned} \tag{B17}$$

For a weak pairing superconductor, the energy scale of the gap functions  $\psi(\mathbf{k})$  and  $|\mathbf{d}(\mathbf{k})|$  is much smaller than that of  $\varepsilon(\mathbf{k})$  and  $|\mathbf{g}(\mathbf{k})|$ . Thus we can rescale  $\psi(\mathbf{k})$  and  $\mathbf{d}(\mathbf{k})$  as  $a\psi(\mathbf{k})$  and  $a\mathbf{d}(\mathbf{k})$  with a positive small constant  $a$  without changing the value of  $W(k_y)$ . Then for  $a \ll 1$ , it is found that only the neighborhood of the zeros of  $\varepsilon^2(\mathbf{k}) - \mathbf{g}^2(\mathbf{k})$  contributes to  $W(k_y)$ . As a result, in a similar manner to Appendix B 1, we obtain the formula (52).

## Appendix C: $\mathbf{Z}_2$ topological number

First consider the quasi-particle wave function  $|u_n(\mathbf{k})\rangle$  with

$$\mathcal{H}(\mathbf{k})|u_n(k_x, k_y)\rangle = E_n(\mathbf{k})|u_n(k_x, k_y)\rangle. \quad (\text{C1})$$

From the symmetry (75), we can say that if  $|u_n(\mathbf{k})\rangle$  is a quasiparticle state with positive energy  $E_n(\mathbf{k}) > 0$ , then  $C'|u_n^*(-k_x, k_y)\rangle$  is a quasiparticle state with negative energy  $-E_n(-k_x, k_y) < 0$ . (See Eq.(75) for the definition of  $C'$ .) Thus we use a positive (negative)  $n$  for  $|u_n(k_x, k_y)\rangle$  to represent a positive (negative) energy quasiparticle state, and set

$$|u_{-n}(k_x, k_y)\rangle = C'|u_n^*(-k_x, k_y)\rangle. \quad (\text{C2})$$

For the ground state in a superconductor, the negative states are occupied.

Now we introduce the following “gauge field”  $A_x^{(\pm)}(\mathbf{k})$ ,

$$A_x^{(\pm)}(\mathbf{k}) = i \sum_{n \geq 0} \langle u_n(\mathbf{k}) | \partial_{k_x} u_n(\mathbf{k}) \rangle. \quad (\text{C3})$$

From (C2), the gauge field  $A_x^{(\pm)}(\mathbf{k})$  satisfies

$$A_x^{(+)}(k_x, k_y) = A_x^{(-)}(-k_x, k_y). \quad (\text{C4})$$

We also find that  $A_x(\mathbf{k}) = A_x^{(+)}(\mathbf{k}) + A_x^{(-)}(\mathbf{k})$  is given by a total derivative of a function. To see this, we rewrite  $|u_n(\mathbf{k})\rangle$  in a component,

$$|u_n(\mathbf{k})\rangle = \begin{pmatrix} u_n^1(\mathbf{k}) \\ u_n^2(\mathbf{k}) \\ u_n^3(\mathbf{k}) \\ u_n^4(\mathbf{k}) \end{pmatrix}, \quad (\text{C5})$$

and introduce the following  $4 \times 4$  unitary matrix  $V(\mathbf{k})$

$$V_{mn}(\mathbf{k}) = u_n^m(\mathbf{k}), \quad (m = 1, 2, 3, 4, n = 2, 1, -1, -2). \quad (\text{C6})$$

Then  $A_x(\mathbf{k})$  is written as

$$A_x(\mathbf{k}) = i \text{tr}(V^\dagger(\mathbf{k}) \partial_{k_x} V(\mathbf{k})) = i \partial_{k_x} \ln \det V(\mathbf{k}). \quad (\text{C7})$$

In a similar manner as in Ref.<sup>67</sup>, we introduce the  $\mathbf{Z}_2$  topological number  $(-1)^{\nu(k_y)}$  as

$$\nu(k_y) = \frac{1}{\pi} \int_{-\infty}^{\infty} dk_x A_x^{(-)}(k_x, k_y). \quad (\text{C8})$$

Here we regulate the gap function as  $\hat{\Delta}(\mathbf{k}) \rightarrow 0$  far apart from the Fermi surface to define the topological number. Eqs. (C4) and (C7) lead to

$$\begin{aligned}\nu(k_y) &= \frac{1}{\pi} \int_{-\infty}^0 dk_x A_x^{(-)}(k_x, k_y) + \frac{1}{\pi} \int_0^{\infty} dk_x A_x^{(-)}(k_x, k_y) \\ &= \frac{1}{\pi} \int_0^{\infty} dk_x [A_x^{(+)}(k_x, k_y) + A_x^{(-)}(k_x, k_y)] \\ &= \frac{i}{\pi} \ln \left[ \frac{\det V(\infty, k_y)}{\det V(0, k_y)} \right],\end{aligned}\tag{C9}$$

thus, we obtain

$$(-1)^{\nu(k_y)} = \frac{\det V(0, k_y)}{\det V(\infty, k_y)}.\tag{C10}$$

We can see that the right hand side of (C10) indeed takes a  $\mathbf{Z}_2$  value: From Eq.(C2),  $V(0, k_y)$  is given by

$$V(0, k_y) = (|u_2(0, k_y)\rangle, |u_1(0, k_y)\rangle, C'|u_1^*(0, k_y)\rangle, C'|u_2^*(0, k_y)\rangle),\tag{C11}$$

thus it satisfies

$$C'V(0, k_y) = (C'|u_2(0, k_y)\rangle, C'|u_1(0, k_y)\rangle, |u_1^*(0, k_y)\rangle, |u_2^*(0, k_y)\rangle).\tag{C12}$$

Calculating the determinants of both sides, we obtain  $\det V(0, k_y) = \det V^*(0, k_y)$ . This implies  $\det V(0, k_y) = \pm 1$  since  $V(0, k_y)$  is a unitary matrix. In a similar manner, we obtain  $\det V(\infty, k_y) = \pm 1$  from the regularization in which  $k_x = \infty$  and  $k_x = -\infty$  are identified. So the right hand side of (C10) takes  $\pm 1$ .

Using the explicit form of the quasiparticle wave functions of (49), we obtain

$$\det V(0, k_y) = -\text{sgn}[(k_y^2/2m - \mu)^2 - (\lambda k_y)^2]\tag{C13}$$

for the  $d_{xy} + p$ -wave superconductor. Furthermore, due to the regularization of  $\hat{\Delta}(\mathbf{k})$ , we find that  $\mathcal{H}(\mathbf{k})$  is almost diagonal at  $k_x = \infty$ . Thus we have  $|u_2(\infty, k_y)\rangle \sim {}^T(1, 0, 0, 0)$ , and  $|u_1(\infty, k_y)\rangle \sim {}^T(0, 1, 0, 0)$ , which implies  $\det V(\infty, k_y) = -1$ . Therefore, the  $\mathbf{Z}_2$  topological number is evaluated as

$$(-1)^{\nu(k_y)} = \text{sgn}[(k_y^2/2m - \mu)^2 - (\lambda k_y)^2].\tag{C14}$$

Note that there are two differences between the above  $\mathbf{Z}_2$  topological number and that in Ref.<sup>67</sup>. First, the  $\mathbf{Z}_2$  topological number (C8) is defined for any  $k_y$ , while the  $\mathbf{Z}_2$  topological

number in Ref.<sup>67</sup> is defined only for the time-reversal invariant  $k_y$ . This difference comes from the difference in the symmetry we used. In contrast to the  $\mathbf{Z}_2$  topological number in Ref.<sup>67</sup>, where the particle-hole symmetry (6) was used, in order to define (C8), we assume the one-dimensional particle-hole symmetry (75) which requires a special symmetry of gap function such as  $d_{xy} + p$ -wave pairings. Since the  $\mathbf{Z}_2$  topological number in Ref.<sup>67</sup> is available only for the discrete values of  $k_y$ , it cannot explain the existence of the ABS with flat dispersion, although the  $\mathbf{Z}_2$  topological number (C8) can. Second, the line integral in (C8) performed from  $k_x = 0$  to  $k_y = \infty$  as we consider the continuum model of the  $d_{xy} + p$ -wave superconductor.

Even in the presence of the Zeeman magnetic field  $H_y$  in the  $y$ -direction, the symmetry (75) persists in the  $d_{xy} + p$ -wave superconductor. Thus, the  $\mathbf{Z}_2$  topological number can be defined in the same manner as above. The resultant  $\mathbf{Z}_2$  number is

$$(-1)^{\nu(k_y)} = \text{sgn}[(k_y^2/2m - \mu)^2 - (\lambda k_y)^2 - (\mu_B H_y)^2]. \quad (\text{C15})$$

#### Appendix D: Relation to the odd-frequency pairing amplitude generated at the surface

In this appendix, we would like to discuss the relevance of Andreev bound state and odd-frequency pairing function in more detail<sup>49,51,52</sup>. It has been clarified that inhomogeneity of superconductivity can induce odd-frequency pairing function<sup>49,51,52,131–134</sup>. For this purpose, it is better to use quasi classical Green's function, where atomic scale oscillation is removed out<sup>135–143</sup>. Here, we assume Cooper pair with  $S_z = 0$  for simplicity.

First, we consider two-dimensional semi-infinite superconductor in  $x > 0$  where flat surface is located at  $x = 0$ . In the following discussion, to express the symmetry of the frequency dependence of Cooper pair explicitly, we use Matsubara frequency. Quasiclassical Green's function can be written as

$$\hat{g}_+ = \begin{pmatrix} g_+ & f_+ \\ \bar{f}_+ & -g_+ \end{pmatrix} = \begin{pmatrix} 1 + D_+ F_+ & 2iF_+ \\ 2iD_+ & -(1 + D_+ F_+) \end{pmatrix} / (1 - D_+ F_+), \quad (\text{D1})$$

$$\hat{g}_- = \begin{pmatrix} g_- & f_- \\ \bar{f}_- & -g_- \end{pmatrix} = \begin{pmatrix} 1 + D_- F_- & -2iD_- \\ -2iF_- & -(1 + D_- F_-) \end{pmatrix} / (1 - D_- F_-), \quad (\text{D2})$$

by using Riccati parameterization where  $g$  and  $f(\bar{f})$  are normal and anomalous Green's functions, respectively. The subscript  $+$ ( $-$ ) denotes the right and left going quasiparticles. The above Riccati parameters  $D_{\pm}$  and  $F_{\pm}$  obey the following equations,

$$\begin{aligned} v_{Fx} \partial_x D_{\pm} &= -\Delta_{\pm}(1 - D_{\pm}^2) + 2\omega_n D_{\pm}, \\ v_{Fx} \partial_x F_{\pm} &= -\Delta_{\pm}(1 - F_{\pm}^2) - 2\omega_n F_{\pm}. \end{aligned} \quad (\text{D3})$$

The bulk solution of  $D_{\pm}$  for  $x > 0$  can be written as

$$D_{\pm} = \frac{\Delta_{\pm}}{\omega_n + \sqrt{\Delta_{\pm}^2 + \omega_n^2}}. \quad (\text{D4})$$

Here,  $\Delta_{\pm}$  is a pair potential felt by quasiparticle for each trajectory.  $v_{Fx}$  denotes the  $x$ -component of Fermi velocity with  $v_{Fx} \geq 0$ . For bulk  $d_{xy}$ -wave superconductor, it is given by

$$\Delta_{\pm} = \frac{\pm k_x k_y}{k^2} \Delta_0,$$

for  $k_x \geq 0$ . On the other hand, the corresponding quantity for  $p_x$ -wave, it is given by

$$\Delta_{\pm} = \frac{\pm k_x}{\sqrt{k^2}} \Delta_0,$$

for  $k_x \geq 0$ .

At the surface  $x = 0$ ,  $F_+ = -D_-$  and  $F_- = -D_+$  are satisfied due to the specular reflection. Also in the presence of ABS,  $D_+ = -D_-$  are satisfied. Thus, we obtain

$$f_+ = f_- = \frac{2iD_+}{1 - D_+^2}. \quad (\text{D5})$$

Since  $D_+(-\omega_n) = 1/D_+(\omega_n)$  is satisfied, we can show that  $f_+$  and  $f_-$  is an odd-function of Matsubara frequency  $\omega_n$ . This means that a purely odd-frequency pairing state is realized at the surface in these two cases.

In order to clarify the parity of the pairing, we define pairing amplitude which is available both for positive and negative  $k_x$ . We write explicitly the  $\mathbf{k}$  dependence of the pairing amplitude. We introduce  $f(k_x, k_y)$  as  $f(k_x, k_y) = f_+(k_x, k_y)$  and  $f(-k_x, k_y) = f_-(k_x, k_y)$  for  $k_x \geq 0$ . For even-parity pairing,  $f(k_x, k_y) = f(-k_x, -k_y)$  is satisfied. On the other hand, for odd-parity case,  $f(k_x, k_y) = -f(-k_x, -k_y)$  is satisfied. Here, let us discuss the parity of the odd-frequency pairings obtained above. For  $d_{xy}$ -wave pair potential, since  $f_-(k_x, k_y) = -f_-(k_x, -k_y)$  is satisfied, it is straightforward to derive that  $f(k_x, k_y) = -f(-k_x, -k_y)$

is satisfied. This means the realization of odd-parity pairing in this case. For  $p_x$ -wave pair potential, since  $f_-(k_x, k_y) = f_-(k_x, -k_y)$  is satisfied, it is easy to see that  $f(k_x, k_y) = f(-k_x, -k_y)$  is satisfied. This means the generation of even-parity pairing in this case.

To see concrete form of  $f(k_x, k_y)$ , we neglect the spatial dependence of  $\Delta_{\pm}$ . Then,  $f_{\pm}$  is given by

$$f_+ = f_- = \frac{i\Delta_0}{\omega_n} \frac{k_x k_y}{\mathbf{k}^2}, \quad (\text{D6})$$

for  $d_{xy}$ -wave pairing and

$$f_+ = f_- = \frac{i\Delta_0}{\omega_n} \frac{k_x}{\sqrt{\mathbf{k}^2}}, \quad (\text{D7})$$

for  $p_x$ -wave pairing. The resulting  $f(k_x, k_y)$  is given by

$$f(k_x, k_y) = \frac{i\text{sgn}(k_x)\Delta_0}{\omega_n} \frac{k_x k_y}{\mathbf{k}^2} = \frac{i\text{sgn}(k_y)\Delta_0}{\omega_n} \frac{|k_x| |k_y|}{\mathbf{k}^2}, \quad (\text{D8})$$

for  $d_{xy}$ -wave pair potential, and

$$f(k_x, k_y) = \frac{i\text{sgn}(k_x)\Delta_0}{\omega_n} \frac{k_x}{\sqrt{\mathbf{k}^2}} = \frac{i\Delta_0}{\omega_n} \frac{|k_x|}{\sqrt{\mathbf{k}^2}}, \quad (\text{D9})$$

for  $p_x$ -wave pairing. It is evident that odd-frequency odd-parity pairing in the former case and odd-frequency even-parity pairing in the latter case are realized. This is consistent with the fact that the spin of Cooper pairing is conserved. The difference of the parity results in a remarkable difference when we consider proximity effect into DN attached to superconductor<sup>49,51,52</sup>.

In DN, only  $s$ -wave even parity pairing is possible due to impurity scattering. Thus, odd-parity odd-frequency pairing amplitude cannot penetrate into DN. Thus, for  $d_{xy}$ -wave superconductor, ABS cannot enter into DN since it is expressed by odd-frequency spin-singlet odd-parity state. On the other hand, for  $p_x$ -wave superconductor, ABS can enter into DN since it is expressed by odd-frequency spin-singlet even-parity state including  $s$ -wave channel. Thus, it has been shown that proximity effect of  $d_{xy}$ -wave superconductor and  $p_x$ -wave superconductor is completely different<sup>44-48</sup>.

Next, we consider a two-dimensional semi-infinite superconductor in  $x < 0$  where flat surface is located at  $x = 0$ . Quasiclassical Green's function can be written as

$$\hat{g}_+ = \begin{pmatrix} g_+ & f_+ \\ \bar{f}_+ & -g_+ \end{pmatrix} = \begin{pmatrix} 1 + D_+ F_+ & -2iD_+ \\ -2iF_+ & -(1 + D_+ F_+) \end{pmatrix} / (1 - D_+ F_+), \quad (\text{D10})$$



$$\hat{g}_- = \begin{pmatrix} g_- & f_- \\ \bar{f}_- & -g_- \end{pmatrix} = \begin{pmatrix} 1 + D_- F_- & 2iF_- \\ 2iD_- & -(1 + D_- F_-) \end{pmatrix} / (1 - D_- F_-), \quad (\text{D11})$$

by using Riccati parameterization. The subscript  $+$ ( $-$ ) again denotes the right and left going quasiparticles. Following the similar discussion in the case where two-dimensional semi-infinite superconductor is located on  $x > 0$ , we can use the relation  $D_+ = -F_-$  and  $D_+ = -F_+$ . In the presence of Andreev bound state (ABS),  $D_+ = -D_-$  are satisfied. Then, we can write

$$f_+ = \frac{-2iD_+}{1 - D_+^2}. \quad (\text{D12})$$

If we neglect the spatial dependence of  $\Delta_{\pm}$ ,  $f_{\pm}$  is given by

$$f_+ = f_- = \frac{-i\Delta_0}{\omega_n} \frac{k_x k_y}{\mathbf{k}^2}, \quad (\text{D13})$$

for spin-singlet  $d_{xy}$ -wave pairing and

$$f_+ = f_- = \frac{-i\Delta_0}{\omega_n} \frac{k_x}{\sqrt{\mathbf{k}^2}}, \quad (\text{D14})$$

for spin-triplet  $p_x$ -wave pairing. Following similar discussions below Eq. (D6),  $f(k_x, k_y)$  is given by

$$f(k_x, k_y) = -\frac{i\text{sgn}(k_x)\Delta_0}{\omega_n} \frac{k_x k_y}{\mathbf{k}^2} = -\frac{i\text{sgn}(k_y)\Delta_0}{\omega_n} \frac{|k_x| |k_y|}{\mathbf{k}^2}, \quad (\text{D15})$$

for spin-singlet  $d_{xy}$ -wave and

$$f(k_x, k_y) = -\frac{i\text{sgn}(k_x)\Delta_0}{\omega_n} \frac{k_x}{\sqrt{\mathbf{k}^2}} = -\frac{i\Delta_0}{\omega_n} \frac{|k_x|}{\sqrt{\mathbf{k}^2}}, \quad (\text{D16})$$

for spin-triplet  $p_x$ -wave.

## Appendix E: diagonalization of $\hat{q}(\mathbf{k}, x)$

Let us consider an  $N \times N$  matrix  $\hat{q}(\mathbf{k}, x)$  with eigenvalues  $\lambda_1, \dots, \lambda_N$ . Then we have two kinds of eigenvectors : The first one is right eigenvectors,

$$\hat{q}(\mathbf{k}, x)a_n(\mathbf{k}, x) = \lambda_n(\mathbf{k}, x)a_n(\mathbf{k}, x), \quad (\text{E1})$$

and the second one is left eigenvectors

$$b_n^\dagger(\mathbf{k}, x)\hat{q}(\mathbf{k}, x) = b_n^\dagger(\mathbf{k}, x)\lambda_n(\mathbf{k}, x), \quad (\text{E2})$$

with the normalization condition

$$b_n^\dagger(\mathbf{k}, x)a_m(\mathbf{k}, x) = \delta_{mn}. \quad (\text{E3})$$

Note that  $a_n(\mathbf{k}, x) \neq b_n(\mathbf{k}, x)$  in general unless  $\hat{q}(\mathbf{k}, x)$  is a hermitian matrix. Eqs.(E1) and (E2) lead to

$$\begin{aligned} \hat{q}(\mathbf{k}, x)A(\mathbf{k}, x) &= A(\mathbf{k}, x)\Lambda(\mathbf{k}, x), \\ q^\dagger(\mathbf{k}, x)B(\mathbf{k}, x) &= B(\mathbf{k}, x)\Lambda^*(\mathbf{k}, x), \end{aligned} \quad (\text{E4})$$

with

$$\begin{aligned} A(\mathbf{k}, x) &= (a_1(\mathbf{k}, x), \dots, a_N(\mathbf{k}, x)), \\ B(\mathbf{k}, x) &= (b_1(\mathbf{k}, x), \dots, b_N(\mathbf{k}, x)), \\ \Lambda(\mathbf{k}, x) &= \text{diag}(\lambda_1(\mathbf{k}, x), \dots, \lambda_N(\mathbf{k}, x)). \end{aligned} \quad (\text{E5})$$

Using the normalization condition (E3) which reads

$$B^\dagger(\mathbf{k}, x)A(\mathbf{k}, x) = A^\dagger(\mathbf{k}, x)B(\mathbf{k}, x) = \mathbf{1}_{N \times N}, \quad (\text{E6})$$

we obtain

$$\begin{aligned} \hat{q}(\mathbf{k}, x) &= A(\mathbf{k}, x)\Lambda(\mathbf{k}, x)B^\dagger(\mathbf{k}, x), \\ \hat{q}^\dagger(\mathbf{k}, x) &= B(\mathbf{k}, x)\Lambda^*(\mathbf{k}, x)A^\dagger(\mathbf{k}, x). \end{aligned} \quad (\text{E7})$$

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